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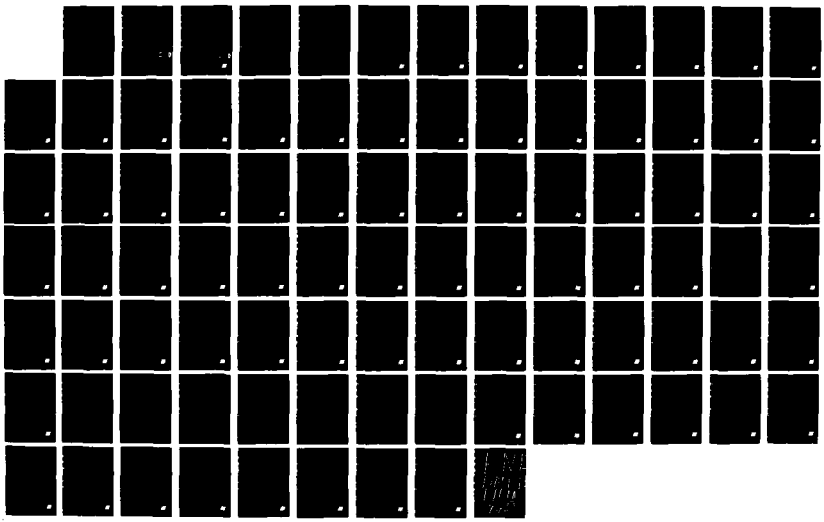

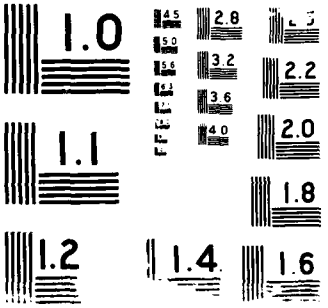
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GC-TR-86-1628-1

EVALUATION OF CETANE INDICES FOR MARINE FUELS

GEO-CENTERS, INC

GC-TR-86-1628-1

EVALUATION OF CETANE INDICES FOR MARINE FUELS

PREPARED FOR
NAVAL RESEARCH LABORATORY
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In this study, 14 cetane indices were evaluated with respect to their correlations with cetane number. Most of the evaluations were performed on a 28 fuel set taken from a worldwide survey of commercial marine fuels obtained in 13 different countries. Cetane numbers of the fuels ranged from 41-57. Of the 14 cetane indices, 9 were published cetane indices and 5 were trial correlations.

The published cetane indices included ASTM D976-80, Ingham et al.'s proposed equation for replacement of D976-80 (their distillation temperatures/density equation), Ingham et al.'s aniline point equation, the Canadian General Standards Board cetane index, the Colling and Unzelman equation, the Ethyl Corp. equation, the SWRI cetane index for fuels containing aromatics, as well as the Diesel Index and ASTM D976-66 for comparison purposes. The trial cetane indices included 4 correlations based on established parameters and 1 correlation based on refractive index and density.

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Evaluations were based on regression analyses of cetane number vs cetane index as well as on the predictability of the cetane indices as defined by arbitrary criteria imposed on the results. Relatively good correlations with cetane number were observed for most of the cetane indices that were based on distillation temperature(s) and density ($R^2 = \sim 0.8$). The lowest correlation with cetane number was exhibited by a trial cetane index that was based on refractive index and density ($R^2 = 0.45$, for 26 of the 28 fuel set).

ASTM D976-80 exhibited the lowest % overprediction but exhibited a tendency to underpredict on these fuels. Furthermore, none of the cetane indices appear to exhibit significant improvement over ASTM D976-80. However, the most promising of the published cetane indices was Ingham's proposed equation for replacement of D976-80; nevertheless, it exhibited a tendency to overpredict on these fuels. Of the trial correlations, the most promising was the modified ASTM D976-80 cetane index. This equation employs the same formulation as D976-80 but differs from it, in that its mid-distillation temperature term is the average of 10, 50, and 90% distillation temperatures.

CONTENTS

LIST OF TABLES

LIST OF TABLES (CONT'D)

LIST OF TABLES (CONT'D)

LIST OF FIGURES

LIST OF APPENDICES

1.0 INTRODUCTION

The determination of cetane number is important in characterizing the ignition quality of diesel fuels. As stipulated by Military Specification, MIL-F-16884H, cetane number is determined via an engine test method, ASTM D 613 [1]. An approved alternative method, ASTM D 976 [2] involves a predictive equation of cetane number known as the calculated cetane index. This is based on the mid-boiling point and density of the fuel. For purposes of convenience, many refineries rely solely on the D976 method. However, because of problems such as biases [3] and inherent limitations that are associated with both the old [2a] and revised D976 equations [2b], there is need for a cetane index (predictive equation) which gives better correlation between cetane number and cetane index.

Based on a review of the literature [4], 9 published cetane indices were selected for evaluation with respect to their correlations with cetane number. Selection of the indices was based on the merits of their accuracy in predicting the cetane number of the fuel as well as on their simplicity. The historic Diesel Index, which was formulated in 1934 [5], and the old calculated cetane index, D976-66 [2a], were also included among the 9 cetane indices for comparison purposes. Possible development of new correlations based on established parameters as well as on simple measurements such as refractive index and density was also examined.

The fuel set for evaluations of the various cetane indices comprised 33 commercial marine fuels from 13 countries and were obtained from a U.S. Navy worldwide survey conducted in 1983. However, this entire set of fuels was not used in the evaluations because of incomplete data for four fuels. Thus, evaluations of most of the cetane indices were limited to a maximum of 29 fuels.

In a preliminary investigation to determine the correlation of various refractive index/density trial expressions with cetane number, the fuel set involved 26 of the 29 previously mentioned fuel set. However, in the subsequent evaluation of a selected refractive index/density trial cetane index, a maximum of 27 fuels was employed.

2.0 EXPERIMENTAL

2.1 Fuels

2.1.1 Classification

Based on the classification and composition given by the suppliers, the 33 commercial marine fuels comprised the following [6]:

a) 19 marine gas oils (100% distillate products).
b) 8 heavy marine gas oils (approximately 100% distillates but may contain up to 0.5 volume % residual contamination).
c) 6 marine diesel fuels (mid-distillates typically containing less than 10 volume % residuum).

Note, although some of the fuels were found to be mis-classified, they were not re-classified after analysis [6].

2.1.2 Properties

A detailed description of the fuels including a list of their physical and chemical properties has been documented by Burnett et al. [6]. Nevertheless, for convenience purposes, a brief description of the fuels is given in Table 1. The properties employed in the determination of the various cetane indices and their measured values for the respective fuels are listed in Tables 2A, and 2B. Much of the data listed in Tables 1, 2A, and 2B were taken from the paper by Burnett et al. [6].

Exceptions include the distillation temperatures data, which were obtained, in deg F, via private communication from Sun Refining and Marketing Co., Pennsylvania (see Table 2A). This Company had performed all the analyses listed in Burnett et al.'s paper [6]. Conversion of the distillation temperatures data from deg F to deg C were made at the Naval Research Laboratory (NRL); likewise, the conversion of API gravity measurements to density. The latter conversion was performed using the formula given in ASTM D287 [7] (see Appendix B1.1.1, No.1b). The refractive index data, included in Table 2B, are recent measurements and were made by Geo-Centers Inc., at the Naval Research Laboratory (see Section 2.2.2.2).

Additional aniline point data (see Table 2B) were also obtained for six fuels from the National Institute for Petroleum and Energy Research (NIPER, Oklahoma). Four of the six fuels were first-time determinations. Their aniline points had not been determined by Sun Refining and Marketing Co., possibly because they were classified as marine diesel fuels. The remaining two fuels were repeats of those determined by the Sun Co., for comparison purposes. Aniline point data for the repeat fuels by NIPER were in agreement with Sun Company's data within 1-2 deg F.

2.1.3 Composition

Compositional analysis of the fuels, according to class structure, is shown in Table 2C. The classes of compounds separated include saturates, monocyclic and dicyclic aromatics, fluorenes, and phenanthrenes. Analysis was

performed by Dorn et al. at the Virginia Polytechnic Institute, Blacksburg, VA., using liquid chromatography/proton nuclear magnetic resonance spectrometry average composition analysis [8].

The data, which were obtained as fractions of total carbon of a specific compound class were converted to weight % by Geo-Centers Inc., at the Naval Research Laboratory (see Appendix D1 for conversion method). It is this converted data, i.e., in wt % that is shown in Table 2C. However, as shown in Appendix D2, the small differences between the measured % of total carbon and the calculated weight % for the 29 fuels examined suggest that the conversion to weight percent may not be necessary.

Compositional analysis, according to proton type, is shown in Table 2D and is based on proton NMR analysis. The % proton type is relative to the total number of protons. Analysis was performed at Southwest Research Institute (SwRI) using a JEOL FX 90Q Fourier Transform NMR spectrometer. The various types of assigned protons and their chemical shifts, which are listed in Appendix C, were taken from the paper by Bailey et al. [9].

Reproducibility of the NMR integrations using SwRI's FIDs (Free Induction Decay) was examined by Geo-Centers Inc., at the Naval Research Laboratory (NRL). Each integration was performed in triplicate and the average values for the various types of assigned protons were used in the calculation of the SwRI cetane index for each fuel (see Appendix E).

2.1.4 Fuel Sets Employed

Except for the refractive index/density correlation determinations with cetane number, the fuel set for all the cetane indices evaluated, comprised a maximum of 29 fuels. This maximum was employed because the data for determination of the various cetane indices were complete for only these fuels.

However, subsequent evaluations of the cetane indices with respect to their correlations with cetane number were performed on a 28 fuel set and to a limited extent, on the 29 fuel set. The 28 set included the same fuels as the 29 except for fuel, 83-10. This fuel was excluded because all the cetane indices of this fuel were found to be significantly and consistently lower than its cetane number.

Possible explanations for the consistently lower cetane indices for this fuel relative to its cetane number include either the presence of an ignition improver, or an error in the determination of its cetane number, or both. Note, to compare the predictability of the various cetane indices, relative to each other, fuel sets containing the same fuels were used in the evaluations.

In a preliminary investigation to determine the correlation of various refractive index/density trial expressions with cetane number, the fuel set comprised 26 of the 28 fuels mentioned previously. The 8 fuel set, referred to earlier, was decreased further because the refractive indices of 2 of these fuels could not be

accurately determined owing to their dark color. However, in the subsequent evaluation of a selected refractive index/density trial cetane index, a maximum of 27 fuels, 83-10 included, was employed.

2.2 Cetane Indices

The indices that were evaluated included selected published cetane indices (see Section 2.2.1) and trial correlations (see Section 2.2.2). The trial correlations comprised those based on established parameters (see Section 2.2.2.1) as well as those based on simple measurements (see Section 2.2.2.2). Lotus 1-2-3 was employed in the determination of the published cetane indices, as well as in the development of new cetane indices, and in the evaluation of all the cetane indices including regression analyses of cetane number vs cetane index.

2.2.1 Selected Published Cetane Indices

Those evaluated are listed below along with the parameters employed in their determinations. (See Appendix A for a list of symbols pertaining to these parameters as well as for the ASTM methods employed in the determination of these parameters; also, see Appendix B for the actual equations).

1. Calculated Cetane Index
   a. **ASTM D 976-66:** Mid-boiling point (deg F) and API Gravity (deg API) [2a].

b. **ASTM D 976-80:** Mid-boiling point (deg C) and density (at 15 deg C, g/mL); or same as (a) above [2b].

2. **Ingham et al.'s Four Variable Equation:** 10, 50, and 90% distillation temperatures (deg C) and density (at 15 deg C, g/mL) [10].

3. **Improvement Equations of ASTM D976-80:** Same parameters as ASTM D 976-80.

   a. Collins and Unzelman Equation [3].
   b. Ethyl Equation [11].

4. **Canadian General Standards Board (CGSB) Cetane Index:** 10, 50, and 90% distillation temperatures (deg C), density (at 15 deg C, g/mL), aniline point (deg C), and viscosity (at 40 deg C, cSt) [12].

5. **Ingham et al.'s Aniline Point Equation:** Aniline Point (deg C) [10].

6. **Diesel Index:** Aniline Point (deg F) and API Gravity (deg API) [5].

7. **Southwest Research Institute (SwRI) Cetane Index:** specific types of protons, wt % hydrogen content, and density (g/mL) [9].

2.2.2 Trial Correlations

2.2.2.1 Based on Established Parameters

Four such cetane indices were examined. These are as follows:

1. A trial cetane index based on aniline point (see Appendix B1.3.2).

2. Three trial cetane indices based on mid-boiling point and density. These include:

   a) Two new correlations (see Appendix B1.1.2) obtained by regression analysis of cetane number vs:

      (i) the mid-boiling point and density parameters

      (ii) the average mid-boiling point* and density parameters

   b) The third trial correlation was a modified form of ASTM D976-80 in which the same D976-80 equation was employed but where the mid-boiling point term was the average mid-boiling point*. This trial cetane index is subsequently referred to as the modified ASTM D976-80.

* Note: the average mid-boiling point refers to the average distillation temperature in deg C of the 10, 50 and 90% recovered distillate.

2.2.2.2 Based on Simple Measurements

Cetane Indices based on refractive index and density were also examined. Refractive index was measured using an Abbe Refractometer, model 10450. An external water circulating bath was used to minimise temperature fluctuations. Measurements were made at 25.1 deg C, although fluctuations to 25.2 deg C were noted. Refractive indices for the fuels measured are included in Table 2B. As indicated in Table 2B, five of the 33 fuels were dark. Consequently, their refractive indices could not be measured accurately.

3.0 RESULTS AND DISCUSSION

3.1 Determination of Published and Trial Cetane Indices Based on Established Parameters

Results of the determination of the various cetane indices are given in Tables 3A - 3C. Specifically, Table 3A lists the results of 5 published cetane indices that are based on distillation temperatures and density only. Table 3B lists the results of three trial correlation indices, which are based on similar parameters; the results of ASTM D976-80 are also included in Table 3B for comparison purposes. Table 3C lists the results of four published cetane indices and 1 trial cetane index, which are based on other conventional parameters. These include API gravity, aniline point, viscosity, and structural composition. Note, in these Tables, cetane indices for the last 4 fuels listed were often not determined because of incomplete data. Subsequent evaluation of the results is given in Section 3.4.

3.2 Determination of the Reproducibility of SwRI Cetane Index

The Southwest Research Institute (SwRI) cetane index determinations, shown in Table 3C, are based on compositional analysis performed at SwRI, using proton NMR spectrometry. Using SwRI's FID (Free Induction Decay) data, reproducibility of the NMR integrations performed at SwRI was examined at NRL for all 33 fuels.

The results (see Table 4), indicate that for the same FID, the numerical differences in cetane indices based on integrations performed at SwRI and at NRL were within the range of 0.1-1.0 in most cases. Differences of approx. 2.0 were observed in only 2 cases. Also, standard deviation of the differences for the 33 fuels was +/- 0.5. This is well within the reproducibility limits allowed by ASTM D613 for cetane number. (Reproduciblity limits allowed are 2.5 to 3.3 for cetane numbers 40 to 56 respectively). Furthermore, results of a regression analysis indicated the reproducibility between the two integration sets was very good (R^2 = 0.992).

3.3 Development of a Cetane Index Based on Simple Measurements

In the development of a cetane index based on simple measurements such as refractive index and density, regression analyses were performed on these parameters using a 26 fuel set (see Section 2.1.4). The various parameters examined included refractive index, density, a combination of both refractive index and density, as well as, 17 other combinations involving various functions of refractive index and density.

The results showed limited promise: Of the various parameters and functions of these parameters investigated, the best was one involving: D^2, RI^2, and RI/D (see Table 5). However, its correlation coefficient was somewhat low (R^2 = 0.448). For a perfect correlation, R^2 = 1. Also, the

errors of their coefficients (i.e., the errors of the slopes of the D^2, RI^2, and RI/D terms in the multiple linear regression equation) were rather high +/- 35%. Its standard error of Y estimate = 3.1 was also somewhat high (this parameter refers to the error in estimating the cetane number). Nevertheless, this trial cetane index (see Appendix B1.5 for its formulation) was employed in evaluating predictability of cetane number.

3.4 Evaluation of Cetane Indices

Evaluation of the various cetane indices was based on the following two methods:

1. The ability to predict the cetane number of fuels.

2. Regression analysis of cetane number versus cetane index.

3.4.1 Evaluation Based on Predictability

3.4.1.1 Determination of Predictability

The following procedure was employed in the determination of the predictability of each cetane index:

1. The numerical difference between cetane index and cetane number for each fuel was first calculated. This difference, i.e., cetane index - cetane number

is defined as the **predictive range.** The results are given in Tables 6A, 6B, and 6C for cetane indices that are based on established parameters, and in Table 7 for the best trial cetane index based on refractive index and density.

2. To qualitatively assess the results, the following arbitrary criteria were adopted:

   a) Cetane indices which differed from their respective cetane numbers within a predictive range of +/-(0 to 2.0) were designated as being predictive of cetane number.

   b) Cetane indices which were lower than their respective cetane numbers within a predictive range of -(2.1 to >5.0) were designated as being underpredictive of cetane number.

   c) Cetane indices which were higher than their respective cetane numbers within a predictive range of +(2.1 to >5.0) were designated as being overpredictive of cetane number.

3. Based on the criteria given in 2. above, the data for a 28 fuel set (see Section 2.1.4) were then evaluated quantitatively as follows:

   a) The frequency of predictions, underpredictions, and overpredictions was determined for specfic predictive ranges (see Tables 8A, 8B, and 8C).

b) % Predictability for the specific predictive ranges were also determined (see Tables 9A, 9B, and 9C).

3.4.1.2 Predictability of Cetane Indices Examined

The total % predictions, overpredictions, and underpredictions for the various cetane indices are summarized in Table 10. In this Table, 13 cetane indices were ranked in order of best to worse primarily, on the % predictions and secondarily, on the % overpredictions. This approach was adopted for two reasons:

1) In evaluating the predictability of the various cetane indices, it is obvious that a high frequency of predictions is desirable.

2) Overpredictions will pose a problem to the consumer, but underpredictions will not.

Note: The refractive index/density trial cetane index, placed at the end of the list, was not ranked in these evaluations because the number of fuels employed in its evaluation was 2 less than was employed for the other cetane indices.

Because of the relatively small number of fuels employed in the fuel set, the cetane indices were not subsequently assessed as being: good, fair, or poor predictors, of cetane

number. Instead, the cetane indices were evaluated on their performance relative to the following:

a) ASTM D976-80 (this may be regarded as the reference cetane index.

b) Ingham et al.'s four variable equation which has been proposed as a replacement for D976-80 (i.e., their 3 distillation temperatures/density cetane index).

c) Each other.

Thus, based on the criteria imposed on the results (see Section 3.4.1.1, Nos.1 and 2) and for this limited set of 28 fuels, the following were observed:

1. The best predictability was exhibited by the modified ASTM D976-80, a trial cetane index (see *NB below). However, its % overpredictions was slightly higher than that of ASTM D976-80. Its predictive performance include 79% predictions, 7% over-predictions, and 14% underpredictions. The results for specific predictive ranges are also shown graphically in Figure 1.

   *NB: In this trial cetane index, the formulation of ASTM D976-80 was unchanged, but the 50% distillation temperature was replaced by the average of the 10, 50, and 90% distillation temperatures.

2. The other two trial cetane indices that were based either on density and mid-boiling point or, on density and the average mid-boiling point (average of 10, 50, and 90%) were not improvements of ASTM D976-80 owing to their higher % overpredictions. However, their predictive performance was similar to each other as well as to Ingham et al.'s proposed equation for replacement of D976-80 (i.e., their four variable equation: 3 distillation temperatures/density cetane index).

3. The predictive performance of Ingham et al.'s four variable equation, which was proposed as a replacement for D976-80, was similar to ASTM D976-80 in their % predictions. However, Ingham et al.'s proposed equation differed from ASTM D976-80 in that their equation exhibited a higher % of overpredictions, whereas ASTM D976-80 exhibited a higher % of **under**predictions (cf, Figures 2 and 3). Consequently, in spite of its greater complexity (see Appendix B1.1.1, No.2), Ingham et al.'s four variable equation does not appear to offer significant improvement over ASTM D976-80 for the set of fuels examined in this work.

4. ASTM D976-80 had the lowest % overpredictions of the cetane indices evaluated (approx. 4%). However, it exhibited a tendency to underpredict on these fuels (approx. 30%).

5. The predictability of Ingham et al.'s aniline point cetane index was similar to their distillation temperatures/density cetane index as well as to a trial cetane index based on aniline point only. Consequently, relative to the trial cetane index based on aniline point, in this limited fuel set, the use of normalization in Ingham's aniline point equation (see Appendix B1.3.1) did not appear to be significantly advantageous with respect to increasing the % predictions and decreasing the % over-predictions.

6. Collins and Unzelman, and the Ethyl Corp. Equations, which were formulated as improvements of D976-80 were not found to be improvements. Furthermore, the Ethyl equation exhibited a tendency to overpredict on these fuels (approx. 32%); whereas, Collins and Unzelman equation exhibited similar tendencies to both overpredict and underpredict on these fuels.

7. The Canadian General Standards Board (CGSB) cetane index was not an improvement over ASTM D976-80, in spite of its greater complexity (see Appendix B1.2) . Furthermore, it exhibited a similar tendency of D976-80 to underpredict on these fuels. Its performance for specific predictive ranges are shown graphically in Figure 4.

8. Cetane indices which performed worse than ASTM D976-80 from the viewpoint of overpredictions (see

arbitrary criteria given in Section 3.4.1.1, Nos. 1 and 2) are as follows:

a) The diesel index, which is based on API gravity and aniline point.

b) The SwRI cetane index, which is based on proton NMR compositional analysis, density, and wt % hydrogen. Its performance for specific predictive ranges are shown graphically in Figure 5.

c) The ASTM D976-66, which is based on API gravity and mid-boiling point.

9. Based on a 26 fuel set, the trial refractive index/density cetane index exhibited a tendency to both underpredict and overpredict on these fuels .

3.4.2 Evaluation Based on Regression Analyses of Cetane Number Vs Cetane Index

Regression analyses of cetane number vs cetane index was performed to determine the goodness of fit of the various cetane indices. Since $R^2 = 1$ represents a perfect correlation between cetane number and cetane index, R^2 values which approach 1 would be desirable.

As described in Section 2.1.4, regression analyses were performed on fuel sets containing 28 and 29 fuels for all

the cetane indices evaluated except for the trial cetane index based on refractive index/density for which the fuel sets were 26 and 27 fuels. The results, shown in Table 11, are ranked in the order of best to worse except for the trial cetane index based on refractive index/density, which was not ranked as explained earlier (see Section 3.4.1.2).

Some general observations are as follows:

1. Ingham's proposed equation for replacement of ASTM D976-80 ranked the highest among the correlations of cetane index with cetane number (R^2 = 0.817 for a 28 fuel set). However, its R^2 value was not much higher than many of the cetane indices that are also based on distillation temperature(s) and density.

2. Cetane indices based only on distillation temperature(s) and density, which showed similarly good correlations with cetane number as Ingham's proposed replacement equation include both ASTM D976-80 and the modified ASTM D976-80 (trial cetane index: see Section 2.2.2.1, No.2b) as well as the improvement equations of D976-80 (Collins and Unzelman equation, and the Ethyl equation). Their R^2 values were approx. 0.80.

3. Other cetane indices based also on distillation temperature(s) and density whose correlations with cetane number were slightly less than those mentioned in 2. above include ASTM D976-66 and two trial cetane indices (R^2 = approx. 0.78). However, their differences do not appear to be significant.

4. The correlation of CGSB cetane index, which is based on 10, 50, and 90% distillation temperatures, density, aniline point and viscosity, was similar to many of the cetane indices that are based only on distillation temperatures and density.

5. The correlations of cetane indices based on distillation temperature(s) and density, with cetane number, were better than corresponding correlations with cetane indices based on the following: aniline point only; proton NMR analysis, density, and hydrogen content (SwRI cetane index); API gravity and aniline point; and refractive index/density.

6. Although not shown in Table 11, for most of the cetane indices, their standard errors of the Y estimate (i.e., of cetane number) were approx. 2.

7. Of the various cetane indices, the trial refractive index/density cetane index exhibited the lowest R^2 value, i.e., 0.448 for a 26 fuel set.

8. As would be expected, R^2 values for the 28 fuel set were higher than their corresponding values for the 29 fuel set (see Section 2.1.4).

3.4.3 Evaluation Based on the Combination of Predictability and Regression Analyses

Table 12 was constructed by combining the results from Table 10 with that of Table 11, but with the exclusion of the regression data for the 29 fuel set. However, in Table 12, the results were re-ranked in the order of best to worse, primarily on their R^2 values and secondarily on their % predictions. Based on the limited set of 28 fuels, the following observations were made:

1. Although Ingham et al.'s proposed replacement equation of ASTM D976-80 ranked the highest in its correlation with cetane number (R^2 = 0.817), its tendency to overpredict on these fuels indicates further studies are required to verify this trend.

2. Based on their R^2 values, ASTM D976-80 was similar to Ingham et al.'s proposed replacement equation. However, based on the % overpredictions, ASTM D976-80 performed better than Ingham et al.'s equation. Nevertheless, D976-80 exhibited a tendency to underpredict on these fuels. A similar tendency of D976-80 to underpredict was observed by British and Australian refiners for their fuels [3].

3. Although the R^2 values for Collins and Unzelman equation and the Ethyl equation were high (approx. 0.81), their % predictions were only approx. 54-60%. Similar anomalies between R^2 values and % predictions were also observed for other cetane

indices e.g., CGSB cetane index, D976-66, and the SwRI cetane index. Consequently, evaluations based solely on R^2 values can be misleading.

4. Of the trial cetane indices investigated, the modified ASTM D976-80 (see Section 2.2.2.1, No.2b) appears the most promising as a predictor of cetane number.

5. In general, cetane indices that are based on distillation temperature(s) and density appear to be better predictors of cetane number than those based on API gravity and aniline point (e.g., Diesel index), refractive index and density (trial index), and proton NMR analysis (SwRI cetane index: see also 7. below).

6. The better predictability of cetane indices that are based on distillation temperature(s) and density compared with other parameters mentioned in 5. above, are likely due to distillation temperatures(s) and density being related to aromatic/paraffinic content, the degree of branchiness of the molecules, and to molecular size [13, 14].

7. The relatively poor performance of the SwRI cetane index which is based on proton NMR analysis suggests the need for better compositional analysis, or improved modeling of the SwRI cetane index, or both. In particular, as reported by Glavincevski et al. [15] and Gulder et al [14], the different types of

paraffins, viz, straight and branched chains, are important in the determination of cetane number.

8. As a single predictor, aniline point, which is an indirect measure of aromatic/paraffinic content, appears to correlate well with cetane number (see also Figure 6). This correlation is consistent with the literature [4, 10]. However, the toxicity of aniline disfavours the use of cetane indices involving aniline point.

9. The poor correlation of the refractive index/density trial cetane index with cetane number is likely related to the poor correlation of refractive index of the bulk fuel with cetane number (see Figure 7).

4.0 CONCLUSIONS

The conclusions given below are based on both the predictability of the cetane indices as defined by arbitrary criteria imposed on the results and on regression analyses of cetane number vs cetane index. Unless otherwise stated, the results are based on a fuel set, which comprised 28 commercial marine fuels. These fuels were obtained in 13 different countries during a worldwide survey. Their cetane numbers ranged from approx. 41-57.

1. In general, Ingham et al.'s four variable equation (i.e., three distillation temperatures plus density), which has been proposed as a replacement for ASTM D976-80, was not found to be a significant improvement over D976-80, in spite of using 10, 50, and 90% distillation temperatures as separate parameters in their formulation as well as normalization factors for the distillation temperatures and density parameters. The tendency of Ingham's equation to overpredict on these fuels suggest that further studies are required to verify this observation. Nevertheless, of the published cetane indices, their proposed replacement equation appears to be the most promising.

2. ASTM D976-80 exhibited the lowest % overpredictions of the published and trial cetane indices evaluated. However, it also exhibited a tendency to underpredict on these fuels.

3. Relative to the performance of ASTM D976-80, of the trial cetane indices examined, the modified ASTM D976-80 appears to be the most promising. This index employs the same formulation as D976-80 but differs from it, in that the mid-distillation temperature term employed is the average of the 10, 50, and 90% distillation temperatures instead of the 50% distillation temperature used in ASTM D976-80.

4. The Canadian General Standards Board (CGSB) cetane index was not an improvement over ASTM D976-80 in spite of employing 10, 50, and 90% distillation temperatures as well as 2 additional parameters in its formulation (viz, aniline point and viscosity). Furthermore, it exhibited a tendency similar to D976-80 of underpredicting on these fuels.

5. Cetane indices which exhibited a tendency to overpredict on these fuels include: ASTM D976-66, the SwRI cetane index, and the Diesel Index.

6. Physical properties which appear to contribute to good correlation with cetane number include the combination of distillation temperatures and density. As a single predictor, aniline point is also good. However, the toxicity of aniline disfavors the use of cetane indices involving aniline point.

7. The need for continuing revision of the ASTM D976 method (e.g., D976-66, D976-80, and possibly Ingham et al.'s proposed equation) are indicative of fuel

compositional changes. Consequently, future cetane indices that are based on compositional analysis involving the % straight chain paraffins, % branched chain paraffins, and % aromatics may be better predictors of cetane number than those based on physical properties.

8. The poor performance of the SwRI cetane index, which is based on proton NMR compositional analysis suggests the need for more accurate compositional analysis, improved modeling of the index, or both.

9. A trial cetane index based on refractive index and density did not appear promising. The fuel set employed comprised 26 of the 28 fuel set.

10. Evaluations that are based only on R^2 values can be misleading since this calculation does not define the extent of over- or under-predictions. It is therefore important to also monitor the % predictabilty and especially, the % overpredictions of cetane indices.

5.0 RECOMMENDATIONS

1. Repeat the study on a second set of worldwide survey diesel fuels using the same evaluation methods employed in this study.

2. In the repeat study, eliminate evaluations of the Diesel Index and ASTM D976-66, but perform evaluations of all other cetane indices.

3. To accomplish 1. above, obtain a complete set of data for all the fuels in the second worldwide survey. This should include cetane number, 10, 50, and 90% distillation temperatures, density, aniline point, viscosity, wt % hydrogen, proton NMR analysis and refractive index.

4. Develop new correlations with cetane number based on compositional data.

5. To accomplish 4. above, perform compositional analyses on both sets of worldwide survey diesel fuels with respect to obtaining % straight chain paraffins, % branched chain paraffins, and % aromatics.

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Table 1

Description of Worldwide Survey I Commercial Marine Fuels *

NRL ID	SUPPLIER	ORIGIN	FUEL TYPE	CETANE NO. (ASTM D613)
83-67		Pakistan	MGO	56.6
83-3	Mobil	Tokyo, Japan	HMGO	56.5
83-15	Mobil	Australia 1	MGO	55.2
83-68		Pakistan	MDF	54.6
83-30	B.P.	Sweden 1	MGO	54.6
83-19	Shell	Australia	MGO	54.5
83-72	Caltex	Kenya	MDF	53.8
83-14	Mobil	S. Africa 1	MGO	52.9
83-71	Caltex	Kenya	MGO	52.5
83-69	Exxon	Senegal	MGO	52.4
83-76	Shell	Singapore	HMGO	52.1
83-20	Shell	Australia	HMGO	52.0
83-35	B.P.	England	MGO	51.3
83-17	Mobil	Australia 2	MGO	50.4
83-31	B.P.	Sweden	MDF	50.3
83-22	B.P.	Australia 3	MGO	48.8
83-12	Mobil	East Coast, U.S.	MGO	48.8
83-80	Shell	Jamaica	MGO	48.7
83-36	Caltex	Thailand	MGO	48.7
83-27	Caltex	S. Africa 2	MGO	48.5
83-81	Shell	Jamaica	HMGO	47.8
83-7	Mobil	Tokyo, Japan	MGO	47.7
83-34	B.P.	Sweden 2	MGO	47.3
83-78	Esso	Columbia	MGO	47.1
83-10	Mobil	West Coast, U.S.	MGO	46.8
83-16	Mobil	Australia 1	HMGO	45.7
83-23	B.P.	Australia 2	HMGO	43.6
83-24	B.P.	Australia	MDF	42.8
83-11	Mobil	West Coast, U.S.	HMGO	40.9
83-9	Mobil	Tokyo, Japan	MDF	54.3
83-37	Caltex	Thailand	MDF	50.2
83-74	Shell	Singapore	MGO	48.6
83-26	Caltex	S. Africa	HMGO	47.9

* Fuels are listed in order of decreasing cetane number except for the last 4 fuels. Reason for this separation is due to incomplete data for the last 4 fuels.

Table 2: Characterization of Worldwide Survey I Commercial Marine Fuels

A: API Gravity, Density, and Distillation Temperatures Data

NRL ID	CETANE NO. (ASTM D613)	API GRAVITY	DENSITY	DIST. TEMP. (deg F) 10%	50%	90%	DIST. TEMP. (deg C) 10%	50%	90%
83-67	56.6	36.1	0.8443	496	566	686	258	297	363
83-8	56.5	36.2	0.8438	466	552	642	241	289	339
83-15	55.2	37.8	0.8359	457	520	591	236	271	311
83-68	54.6	32.6	0.8623	508	604	746	264	318	398
83-58	54.6	35.9	0.8453	474	548	646	246	287	341
83-19	54.5	34.5	0.8524	472	540	622	244	282	328
83-72	53.8	30.8	0.8718	546	646	754	286	341	401
83-14	52.9	33.9	0.8555	486	566	666	252	297	352
83-71	52.5	34.8	0.8509	448	560	661	231	293	349
83-69	52.4	34.1	0.8545	478	568	651	248	298	344
83-76	52.1	31.7	0.8670	538	638	716	281	337	380
83-20	52.0	34.6	0.8519	466	540	628	241	282	331
83-35	51.2	36.1	0.8443	428	530	635	220	277	335
83-17	50.4	34.4	0.8529	462	538	654	239	281	346
83-31	50.3	37.1	0.8393	404	520	642	207	271	339
83-22	48.9	32.5	0.8628	458	542	650	237	283	343
83-12	48.8	35.1	0.8493	436	514	596	224	268	313
83-30	48.7	35.8	0.8458	456	519	632	236	271	333
83-26	48.7	31.8	0.8665	483	566	696	251	297	369
83-27	48.5	33.0	0.8602	476	574	678	247	301	359
83-31	47.8	32.8	0.8612	466	550	684	241	288	362
83-7	47.7	36.8	0.8408	434	498	570	223	259	299
83-34	47.3	39.2	0.8289	410	484	560	210	251	293
83-78	47.1	31.4	0.8686	522	586	675	272	308	357
83-10	46.8	30.0	0.8762	432	506	620	222	263	327
83-16	45.7	30.3	0.8745	498	534	606	259	279	319
83-33	42.6	32.2	0.8644	439	523	630	226	273	332
83-24	42.8	27.8	0.8883	484	574	666	251	301	352
83-11	40.9	30.0	0.8762	418	510	648	214	266	342
83-9	54.3	33.7	0.8565	NA	NA	NA	NA	NA	NA
83-37	50.2	32.3	0.8639	NA	NA	NA	NA	NA	NA
83-74	48.6	30.7	0.8724	479	590	NA	249	310	NA
83-26	47.3	31.7	0.8670	NA	NA	Cracked	NA	NA	NA

NA Not Available

Table 2 (Cont'd): Characterisation of Worldwide Survey I Commercial Marine Fuels

8: Aniline Point, Hydrogen Content, Viscosity and Refractive Index Data

NPL ID	CETANE NO. (ASTM D613)	ANILINE POINT deg F	ANILINE POINT deg C	HYDROGEN CONTENT WT. %	VISCOSITY cST @ 40 deg C	REFRACTIVE INDEX @ 25 deg C
83-67	56.6	165.7 ·	74.3	13.54	4.08	1.4714
83-8	56.5	159.5 **	70.8	12.86	3.48	1.4698
83-15	55.2	160.9	71.6	13.27	2.79	1.4666
83-68	54.5	165.5 *	74.2	13.03	5.82	1.4801
83-20	54.6	165.2	74.0	12.71	3.84	1.4705
83-19	54.5	158.0	70.0	13.14	3.31	1.4744
83-72	53.8	169.9 *	76.6	13.08	8.71	Dark
83-14	52.9	158.0	70.0	13.00	4.10	1.4754
83-71	52.5	153.9	67.7	13.31	4.79	1.4755
83-69	52.4	158.9	70.5	13.13	4.37	1.4747
83-75	52.1	168.8	76.0	13.27	6.28	1.4831
83-20	52.0	155.3	68.5	13.04	3.28	1.4778
83-35	51.3	154.2	67.9	13.40	3.06	1.4696
83-17	50.4	155.5	68.6	13.12	3.69	1.4732
83-31	50.3	153.6 *	67.6	13.58	2.93	1.4656
83-22	48.8	150.1	65.6	12.63	3.46	1.4809
83-12	48.3	151.9	66.6	13.21	2.80	1.4721
83-30	48.7	150.4	65.8	13.45	3.06	1.4698
83-36	48.7	154.4	68.0	12.91	4.43	1.4819
83-27	48.5	159.8	70.4	12.96	4.41	1.4797
83-31	47.8	151.5	66.4	13.23	4.18	1.4782
83-7	47.7	145.4	63.0	13.35	2.53	1.4663
83-24	47.2	151.9	66.6	13.50	2.19	1.4596
83-78	47.1	160.4	71.3	13.27	5.84	1.4799
83-10	46.8	129.9	54.4	12.60	3.21	1.4809
83-16	45.7	135.9	57.7	12.95	3.12	1.4993
83-23	43.6	134.7 **	57.2	13.36	2.97	1.4855
83-24	42.8	133.0 *	56.1	12.86	4.18	Dark
83-11	40.9	129.2	53.8	12.89	3.63	1.4811
83-9	54.7	ND	ND	13.25	5.21	Dark
83-37	50.2	ND	ND	12.66	4.81	Dark
83-74	48.6	156.4	69.1	12.92	5.22	1.4846
83-26	47.3	Too Dark	Too Dark	11.60	5.61	Too dark

* Determination by NIPER

** Repeat determination by NIPER (See Section 2.1.2)

ND Not Determined

Table 2 (Cont'd): Characterisation of Worldwide Survey I Commercial Marine Fuels

C: Compositional Analysis *

NRL ID	CETANE NO. (ASTM D613)	SATURATES	MONOCYCLIC AROMATICS	DICYCLIC AROMATICS	FLUORENES	PHENANTHRENES
83-67	56.6	68.49	18.40	8.82	2.77	1.52
83-8	56.5	69.57	18.04	8.56	3.54	0.29
83-15	55.2	76.40	10.16	12.10	1.04	0.29
83-68	54.6	61.76	21.44	11.09	4.00	1.71
83-30	54.6	75.14	15.58	7.30	1.42	0.56
83-19	54.5	68.38	16.53	12.25	1.52	1.32
83-72	53.8	56.25	36.19	5.56	2.00	0.00
83-14	52.9	68.91	19.68	8.47	2.66	0.29
83-71	52.5	62.25	24.43	9.03	2.86	1.43
83-69	52.4	69.37	19.45	7.74	2.00	1.43
83-76	52.1	60.09	28.69	8.76	2.46	0.00
83-17	50.4	69.18	21.75	7.37	1.32	0.38
83-31	50.3	74.19	19.71	4.68	1.23	0.19
83-22	48.8	64.58	16.40	15.69	2.76	0.57
83-12	48.8	67.50	17.64	12.53	1.22	1.12
83-80	48.7	70.76	21.41	7.07	0.76	0.00
83-26	48.7	59.62	21.65	15.58	2.57	0.58
83-27	48.5	70.22	18.17	7.90	2.76	0.95
83-81	47.8	63.12	24.26	9.38	1.62	1.61
83-7	47.7	64.78	25.55	8.72	0.95	0.00
83-24	47.3	74.71	18.85	4.37	1.97	0.10
83-78	47.1	67.25	20.86	8.49	2.17	1.23
83-10	46.8	57.98	34.39	6.86	0.77	0.00
83-23	43.6	61.38	22.02	13.54	1.53	1.52
83-24	42.8	51.90	19.88	20.74	5.09	2.40
83-9	54.3	64.92	20.01	11.32	3.46	0.29
83-37	50.2	65.04	18.75	11.90	3.17	1.24
83-74	48.6	64.93	21.15	11.65	2.28	0.00
83-26	47.8	58.83	24.70	11.48	3.37	1.61

* Performed by Dorn et al. [8], using liquid chromatography/proton NMR spectrometry average compositional analysis. Data available only for fuels listed.

Table 2 (Cont'd): Characterisation of Worldwide Survey I Commercial Marine Fuels

D: Proton NMR Analysis *

NRL ID	CETANE NO. (ASTM D613)	% Proton Type **				
		CH3	CH2	CH	ALPHA	AROMATIC
83-67	56.6	28.46	53.08	7.95	6.41	4.10
83-8	56.5	30.17	50.00	8.10	7.54	4.19
83-15	55.2	28.63	53.53	6.64	6.22	4.98
83-69	54.6	27.75	51.45	8.67	7.51	4.62
83-30	54.6	30.41	48.22	10.41	6.03	4.93
83-19	54.5	27.46	50.15	7.16	8.66	6.57
83-72	53.8	26.94	51.67	9.44	7.50	4.44
83-14	52.9	30.16	49.64	9.24	7.07	4.89
83-71	52.5	29.77	48.49	8.22	9.04	5.48
83-69	52.4	32.28	46.56	10.32	7.14	3.70
83-76	52.1	26.09	50.72	10.72	7.83	4.64
83-20	52.0	25.61	50.91	7.62	9.15	6.71
83-35	51.3	32.67	46.89	10.00	5.78	4.67
83-17	50.4	30.55	45.66	11.90	6.75	5.14
83-31	50.3	31.74	46.85	11.34	6.05	4.03
83-22	48.8	28.70	46.30	9.26	8.95	6.79
83-12	48.8	31.40	44.06	11.35	8.18	5.01
83-80	48.7	34.09	42.68	12.12	7.07	4.04
83-36	48.7	28.81	47.46	10.17	8.23	5.33
83-27	48.3	28.82	46.19	10.00	9.71	5.29
83-81	47.8	33.50	41.75	12.75	7.75	4.25
83-7	47.7	30.25	44.32	9.80	9.80	5.82
83-34	47.3	33.65	45.58	11.22	6.21	3.34
83-78	47.1	33.75	41.81	13.10	7.30	4.03
83-10	46.3	36.88	31.95	16.36	10.13	4.68
83-16	45.7	21.45	48.75	4.18	13.93	11.70
83-23	43.6	25.57	44.54	9.20	12.36	8.33
83-24	42.8	24.77	44.04	9.17	12.54	9.48
83-11	40.9	38.44	32.41	15.83	9.05	4.27
83-9	54.3	28.49	51.28	9.12	7.12	3.99
83-37	50.2	29.03	48.68	9.09	8.21	4.99
83-74	48.6	28.20	45.06	12.50	9.01	5.23
83-26	47.8	32.24	46.10	9.07	8.06	4.53

* Performed by Southwest Research Institute

** Relative to the total number of protons

Table 3: Determination of Cetane Indices

A: Published Cetane Indices That Are Based on Density and Distillation Temperatures *
(Worldwide Survey I Commercial Marine Fuels)

NRL ID	CETANE NO. (ASTM D613)	CCI ASTM D976-66	CCI ASTM D976-80	INGHAM'S DISTN. TEMP./ DENSITY EQN	IMPROVEMENT EQUATIONS OF D976-80	
					ETHYL EQN	COLLINS **
83-67	58.6	59.0	54.6	58.5	58.9	59.0
83-3	58.5	57.2	53.5	55.4	57.2	57.1
83-15	55.2	55.8	52.9	54.9	56.2	56.1
83-68	54.6	57.0	51.7	54.2	54.4	54.2
83-30	54.6	56.1	52.6	55.0	55.8	55.7
83-19	54.5	52.0	49.5	50.9	51.1	50.8
83-72	53.9	58.6	51.1	55.1	53.4	53.2
83-14	52.9	54.5	51.0	53.0	53.3	53.0
83-71	52.5	55.5	51.9	52.1	54.7	54.5
83-69	52.4	55.2	51.5	52.9	54.0	53.8
83-76	52.1	59.5	52.1	56.3	55.0	54.9
83-20	52.0	52.2	49.7	50.9	51.3	51.0
83-35	51.3	53.8	51.1	51.1	53.5	53.3
83-17	50.4	51.5	49.1	50.5	50.5	50.2
83-31	50.3	54.4	51.7	51.2	54.4	54.2
83-22	48.8	48.3	46.5	46.7	46.7	46.4
83-12	48.8	49.4	47.6	47.5	48.3	48.0
83-80	48.7	51.6	49.4	51.2	50.9	50.6
83-36	48.7	50.2	47.6	48.9	48.3	48.0
83-27	48.5	53.8	50.2	51.0	52.1	51.8
83-81	47.8	50.0	47.7	48.7	48.5	48.2
83-7	47.7	50.4	48.4	48.9	49.5	49.2
83-34	47.3	53.0	50.6	51.1	52.8	52.5
83-78	47.1	52.1	48.6	51.6	49.7	49.4
83-10	46.8	38.2	38.5	38.5	36.1	36.4
83-16	45.7	42.8	42.2	43.5	40.8	40.7
83-23	43.6	45.0	43.9	43.6	43.2	43.0
83-24	42.8	43.4	42.1	40.9	40.8	40.7
83-11	40.9	38.3	39.0	38.9	36.7	37.0
83-9	54.7	ND	ND	ND	ND	ND
83-37	50.2	ND	ND	ND	ND	ND
83-74	48.6	51.2	47.7	ND	48.6	48.2
83-25	47.8	ND	ND	ND	ND	ND

* Formulations of these cetane indices are given in Appendix B1.1.1

** Collins and Unzelman Equation

ND Not determined

Table 3: Determination of Cetane Indices

B: Three Trial Cetane Indices That Are Based on Density and Distillation Temperatures (Worldwide Survey I Commercial Marine Fuels)

NRL ID	CETANE NO. (ASTM D613)	Trial Cetane Indices		
		CCI ASTM D976-80	Modified ASTM D976-80 AVG.(MBP) *	LOTUS 1-2-3 REGRESSION ANALYSIS** T50,D	LOTUS 1-2-3 REGRESSION ANALYSIS** AVG.(MBP)*, D
83-67	56.6	54.6	55.9	54.9	56.1
83-8	56.5	53.5	53.6	53.7	53.4
83-15	55.2	52.9	53.2	53.1	52.9
83-68	54.6	51.7	52.6	53.3	54.3
83-30	54.6	52.6	53.4	52.9	53.3
83-19	54.5	49.5	50.0	50.2	50.1
83-72	53.8	51.1	51.2	54.4	54.2
83-14	52.9	51.0	51.5	51.7	51.8
83-71	52.5	51.9	51.6	52.5	51.6
83-69	52.4	51.5	51.3	52.2	51.5
83-76	52.1	52.1	51.8	55.0	53.9
83-20	52.0	49.7	50.1	50.3	50.2
83-35	51.3	51.1	51.2	51.6	51.2
83-17	50.4	49.1	50.5	49.9	50.5
83-31	50.3	51.7	51.9	52.1	51.8
83-22	48.8	46.5	47.2	47.5	47.5
83-12	48.8	47.6	47.8	48.7	48.2
83-80	48.7	49.4	51.2	50.1	51.2
83-36	48.7	47.6	48.8	48.6	49.4
83-27	48.5	50.2	50.3	51.1	50.7
83-81	47.8	47.7	49.2	48.6	49.5
83-7	47.7	48.4	48.8	49.6	49.3
83-34	47.3	50.6	50.7	51.7	51.3
83-78	47.1	48.5	49.1	49.8	50.0
83-10	46.3	38.5	40.1	40.4	40.6
83-16	45.7	42.2	43.4	43.4	43.6
83-23	43.6	43.9	44.8	45.3	45.2
83-24	42.8	42.1	42.2	43.2	42.3
83-11	40.9	39.0	40.8	40.8	41.1
83-9	54.2	ND	ND	ND	ND
83-37	50.2	ND	ND	ND	ND
83-74	48.6	47.7	ND	49.1	ND
83-26	47.8	ND	ND	ND	ND

* AVG.(MBP) = AVG. (T10+T50+T90), deg C

** Formulations of these cetane indices are given in Appendix B1.1.2

ND Not Determined

Table 3: Determination of Cetane Indices

C: Cetane Indices That Are Based on Various Types of Established Parameters *
(Worldwide Survey I Commercial Marine Fuels)

NRL ID	CETANE NO. (ASTM D613)	DIESEL INDEX (G, API)	CGSB EQUATION (T,D,API,VISC)	INGHAM'S ANILINE PT EQN (API)	TRIAL ANILINE PT EQN. (API)	SwRI CETANE INDEX ** (PROTON NMR)
93-67	56.6	59.8	54.9	55.8	54.1	60.3
93-8	56.5	57.7	51.9	52.9	52.1	53.4
93-15	55.2	60.8	52.6	53.5	52.5	59.1
93-68	54.6	54.0	53.5	55.7	54.1	57.2
93-30	54.6	59.3	54.0	55.5	54.0	52.9
93-19	54.5	54.5	50.7	52.3	51.6	54.8
93-72	53.8	52.3	53.6	57.8	55.5	58.5
93-14	52.9	53.6	50.7	52.3	51.6	53.3
93-71	52.5	53.6	48.5	50.5	50.2	52.1
93-69	52.4	54.2	50.9	52.7	51.9	51.1
93-76	52.1	53.5	54.5	57.2	55.2	58.0
93-20	52.0	53.7	49.7	51.1	50.7	55.5
93-35	51.3	55.7	49.5	50.6	50.3	52.3
93-17	50.4	53.5	49.6	51.2	50.7	50.6
93-31	50.3	57.0	49.4	50.3	50.1	52.9
93-22	48.8	48.8	47.2	48.9	48.9	49.2
93-12	48.8	53.3	48.2	49.6	49.5	48.9
93-33	48.7	53.8	48.1	49.0	49.0	47.1
93-36	48.7	49.1	48.7	50.7	50.4	52.1
93-27	48.5	52.4	50.6	52.6	51.8	49.7
93-31	47.8	49.7	47.6	49.5	49.4	45.9
93-7	47.7	53.5	46.3	47.0	47.4	48.1
93-24	47.3	59.5	48.9	49.6	49.5	50.2
93-78	47.1	50.4	50.3	53.3	52.4	46.7
93-10	46.3	39.0	39.3	41.2	42.2	32.5
93-16	45.7	41.2	41.8	43.4	44.2	48.9
93-23	43.6	43.4	41.6	43.3	43.9	46.4
93-24	42.8	37.0	40.0	42.3	43.2	47.4
93-11	40.9	38.6	38.8	40.8	41.8	33.7
93-9	54.3	ND	ND	ND	ND	57.6
93-37	50.2	ND	ND	ND	ND	52.3
93-74	48.6	48.3	ND	51.6	51.3	49.7
93-26	47.3	ND	ND	ND	ND	45.7

* Formulations of these cetane indices are given in Appendix B1.2 - B2

** Based on integrations performed at SwRI

ND Not Determined

Table 4

Evaluation of the Reproducibility of the SwRI Cetane Index
(Worldwide Survey I Commercial Marine Fuels)

NRL ID	CETANE NO. (ASTM D613)	SwRI CETANE INDEX a NRL	SwRI CETANE INDEX b SwRI	DIFFERENCE c,d SwRI CET INDEX NRL - SwRI
83-67	56.6	60.4	60.3	0.1
83-8	56.5	54.3	53.4	0.9
83-15	55.2	60.5	59.1	1.4
83-68	54.6	58.1	57.2	0.9
83-30	54.6	52.7	52.0	0.7
83-19	54.5	56.5	54.8	1.7
83-72	53.8	59.0	58.5	0.5
83-14	52.9	53.8	53.3	0.5
83-71	52.5	53.6	53.1	0.5
83-69	52.4	51.9	51.1	0.8
83-76	52.1	57.9	58.0	-0.1
83-20	52.0	56.0	55.5	0.5
83-35	51.3	53.0	52.3	0.7
83-17	50.4	50.4	50.6	-0.2
83-31	50.3	52.5	52.9	-0.4
83-22	48.8	49.7	49.2	0.5
83-12	48.8	49.2	48.0	1.2
83-80	46.7	48.1	47.1	1.0
83-36	48.7	52.6	52.1	0.5
83-27	48.5	50.6	49.7	0.9
83-81	47.8	47.0	45.9	1.1
83-7	47.7	49.9	48.1	1.8
83-24	47.3	50.2	50.2	0.0
83-78	47.1	47.9	46.7	1.2
83-10	46.8	33.4	32.5	0.9
83-16	45.7	49.9	48.9	1.0
83-23	43.6	49.6	48.4	1.2
83-29	42.3	47.1	47.4	-0.3
83-11	40.9	34.6	33.7	0.9
83-9	54.3	57.7	57.6	0.1
83-77	50.2	53.1	52.3	0.8
83-74	48.6	51.0	49.7	1.3
83-26	47.8	46.8	45.7	1.1

a Based on integrations performed at NRL using SwRI's FIDs: Proton values based on average of triplicate integrations.

b Based on integrations performed at SwRI, using the same FIDs as in a, above

c Standard deviation of the differences is +/- 0.5

d Note: Reproducibility limits allowed by ASTM D613 is 2.5 to 3.3 for cetane numbers, 40 to 56 respectively.

Table 5.

Regression Analyses of Parameter(s) Vs Cetane Number

For Refractive Index / Density And Various Functions of These Parameters

	REGRESSION ANALYSIS FOR 26 FUELS *					
PARAMETERS	R^2	Constant	Std Error of Y Est	X Coeff(s)	Std Error of Coeff	% Error of Coeff
RI	0.148	327.7	3.7	-197.97	92.2	-49
D	0.233	183.6	3.5	-156.00	57.8	-37
D, RI	0.252	22.2	3.5	-257.46	142.4	-56
				168.38	217.1	129
RI Fn ** / D	0.052	-104.5	3.9	489.24	407.3	87
RI^2, 1 / D^2	0.234	-144.3	3.6	44.14	73.8	167
				71.81	44.3	62
RI^2 / D^2	0.243	-51.4	3.5	34.07	12.3	36
D^2, RI^2	0.257	35.4	3.5	-152.58	83.2	-55
				58.00	72.7	125
RI^2 / Log D	0.267	70.4	3.4	0.67	0.2	34
RI / (Log D)	0.270	71.6	3.4	0.98	0.3	34
D^2, RI^2, RI/D	0.448	7200.8	3.1	-4972.20	1750.0	-35
				1641.04	577.9	35
				-4106.72	1489.3	-36
$[RI^2$, (RI^2 / D^2), RI/D,	0.498	29796.2	3.1	788.34	636.3	81
				9346.16	30171.0	323
RI/Log D, $(RI^2$ / Log D)]				-34049.52	110468.5	-324
				62.96	724.0	1152
				-25.89	433.2	-1693

* For 26 of the 28 fuel set taken from Worldwide survey I commercial diesel fuels.

** $RI\ Fn = (n^2 - 1 / n^2 + 2)$

Table 5 (Cont'd)

Regression Analysis of Parameter(s) Vs Cetane Number

For Refractive Index / Density And Various Functions of These Parameters

	REGRESSION ANALYSIS FOR 26 FUELS *					
PARAMETERS **	R^2	Constant	Std Error of Y Est	X Coeff(s)	Std Error of Coeff	% Error of Coeff
RI	0.148	327.7	3.7	-187.97	92.2	-49
D, D^2, RI, RI^2	0.510	-41088.8	3.0	4727.44	13282.0	281
				-3053.94	7667.3	-251
				52730.34	42905.3	81
				-17671.60	14423.3	-82
D, D^2, RI, RI^2, D(RI)	0.510	-40853.6	3.0	5214.53	63224.2	1212
				-2912.42	19584.1	-672
				52125.87	88343.1	169
				-17023.80	46499.2	-269
				-494.15	62642.0	-12677
D, D^2, RI, RI^2, D(Log RI)	0.510	-41378.1	3.0	4991.50	14480.0	29e
				-2472.72	19379.4	-784
				52003.27	49233.1	95
				-16841.50	29301.6	-174
				-6855.52	208955.3	-3049
$(EXP\ RI)^2$/D	0.037	111.7	3.9	-5.94	6.1	-104
EXP (RI)	0.149	238.5	3.7	-43.02	21.0	-49
D^2, EXP (RI)	0.232	-174.6	3.6	71.25	44.7	63
				29.09	49.6	170
D-N, RI-N	0.252	50.2	3.5	-257.46	143.4	-56
				168.38	217.1	129
D-N, RI-N, RI Log D	0.474	260.1	3.0	1299.62	526.5	41
				325.65	193.3	59
				9.68	3.2	33
D-N, RI-N, $(D-N)^2$, $(RI-N)^2$	0.510	51.5	3.1	-488.70	224.2	-46
				599.06	400.5	67
				-3053.94	7667.3	-251
				-17671.60	14423.3	-82

* For 26 of the 28 fuel set taken from Worldwide survey I commercial diesel fuels

** The suffix, -N, of the last three entries refers to normalization, which was performed by subtracting from each observed value, the mean of that term.

Table 6: Numerical Differences Between Cetane Index and Cetane Number

A: For Published Cetane Indices That Are Based on Density and Distillation Temperatures *
(Worldwide Survey I Commercial Marine Fuels)

		Predictive Range: Cetane Index - Cetane Number				
					IMPROVEMENT EQUATIONS OF D976-80	
NRL ID	CETANE NO. (ASTM D613)	CCI ASTM D976-66	CCI ASTM D976-80	INGHAM'S DISTN. TEMP. DENSITY EQN	ETHYL EQN	COLLINS **
87-67	56.6	2.4	-2.0	1.9	2.3	2.4
87-8	56.5	0.7	-3.0	-1.1	0.7	0.6
87-15	55.2	0.6	-2.3	-0.3	1.0	0.9
87-68	54.6	2.4	-2.9	-0.4	-0.2	-0.4
87-20	54.6	1.5	-2.0	0.4	1.2	1.1
87-19	54.5	-2.5	-5.0	-3.6	-3.4	-3.7
87-72	53.8	4.8	-2.7	1.3	-0.4	-0.6
87-14	52.9	1.6	-1.9	0.1	0.4	0.1
87-71	52.5	3.0	-0.6	-0.4	2.2	2.0
87-69	52.4	2.9	-0.9	0.5	1.6	1.4
87-76	52.1	7.4	0.0	4.2	2.9	2.8
87-10	52.0	0.2	-2.3	-1.1	-0.7	-1.0
87-75	51.3	2.5	-0.2	-0.2	2.2	2.0
87-17	50.4	1.1	-1.3	0.1	0.1	-0.2
87-31	50.3	4.1	1.4	0.9	4.1	3.9
87-22	48.3	-0.5	-2.3	-2.1	-2.1	-2.4
87-12	48.3	0.6	-1.2	-1.3	-0.5	-0.8
87-80	48.7	2.9	0.7	2.5	2.2	1.9
87-26	48.7	1.5	-1.1	0.2	-0.4	-0.7
87-27	48.3	5.3	1.7	2.5	3.6	3.3
87-91	47.8	2.2	-0.1	0.9	0.7	0.4
87-7	47.7	2.7	0.7	1.2	1.9	1.6
87-24	47.3	5.7	3.3	3.8	5.5	5.2
87-73	47.1	5.0	1.4	4.5	2.6	2.3
87-10	46.9	-8.6	-8.3	-8.3	-10.7	-10.4
87-16	45.7	-2.9	-3.5	-2.2	-4.9	-5.0
87-23	43.6	1.4	0.3	0.0	-0.4	-0.6
87-24	42.8	0.6	-0.7	-1.9	-2.0	-2.1
87-11	40.9	-2.1	-1.9	-2.0	-4.2	-3.9
87-9	54.3	ND	ND	ND	ND	ND
87-27	53.2	ND	ND	ND	ND	ND
87-74	48.6	2.6	-0.9	ND	-0.1	-0.4
87-25	47.8	ND	ND	ND	ND	ND

* Formulations of these cetane indices are given in Appendix B1.1.1

** Collins and Unzelman Equation

Table 6: Numerical Differences Between Cetane Index and Cetane Number

B: For Three Trial Cetane Indices That Are Based on Density and Distillation Temperatures (Worldwide Survey I Commercial Marine Fuels)

		Predictive Range: Cetane Index - Cetane Number			
			Trial Cetane Indices		
NRL ID	CETANE NO. (ASTM D613)	CCI ASTM D976-80	Modified ASTM D976-80 AV(MBP) *	LOTUS 1-2-3 REGRESSION ANALYSIS** T50,D	AVG.(MBP)*,D
80-67	56.6	-2.0	-0.7	-1.7	-0.5
80-8	56.5	-3.0	-2.9	-2.8	-3.1
80-15	55.2	-2.3	-2.0	-2.1	-2.3
80-69	54.6	-2.9	-2.0	-1.3	-0.3
80-70	54.6	-2.0	-1.2	-1.7	-1.3
80-19	54.5	-5.0	-4.5	-4.3	-4.4
80-72	53.8	-2.7	-2.6	0.6	0.4
80-14	52.9	-1.9	-1.4	-1.2	-1.1
80-71	52.5	-0.6	-0.9	0.0	-0.9
80-65	52.4	-0.9	-1.1	-0.2	-0.9
80-76	52.1	0.0	-0.3	2.9	1.8
80-20	52.0	-2.3	-1.9	-1.7	-1.8
80-05	51.3	-0.2	-0.1	0.3	-0.1
80-17	50.4	-1.3	0.1	-0.5	0.1
80-21	50.3	1.4	1.6	1.8	1.5
80-22	48.3	-2.3	-1.6	-1.3	-1.3
80-12	48.3	-1.9	-1.0	-0.1	-0.6
80-80	48.1	0.7	2.5	1.4	2.5
80-26	48.1	-1.1	0.1	-0.1	0.7
80-27	46.5	1.7	1.8	2.6	2.2
80-81	47.3	-0.1	1.4	0.8	1.7
80-7	47.1	0.7	1.1	1.9	1.6
80-24	47.3	3.3	3.4	4.4	4.0
80-78	47.1	1.4	2.0	2.7	2.9
80-10	46.3	-6.3	-6.7	-6.4	-6.2
80-16	45.7	-3.5	-2.3	-2.3	-2.1
80-23	42.6	0.3	1.2	1.7	1.6
80-25	42.3	-0.7	-0.6	0.4	-0.5
80-11	40.9	-1.9	-0.1	-0.1	0.2
80-9	54.0	ND	ND	ND	ND
80-27	50.2	ND	ND	ND	ND
80-74	48.6	-0.9	ND	0.5	ND
80-05	47.3	ND	ND	ND	ND

* AVG.(MBP) = AVG. (T10+T50+T90), deg C

** Formulations of these cetane indices are given in Appendix B1.1.2

Table 6: Numerical Differences Between Cetane Index and Cetane Number

C: For Cetane Indices That Are Based on Various Types of Established Parameters[a]
(Worldwide Survey I Commercial Marine Fuels)

		Predictive Range: Cetane Index - Cetane Number					
						SwRI CETANE INDEX (PROTON NMR ANALYSIS)	
NRL ID	CETANE NO. (ASTM D613)	DIESEL INDEX (G, AP)	CGSB EQUATION (T,D,AP,VISC)	INGHAM'S ANILINE PT EQN (AP)	TRIAL ANILINE PT EQN (AP)	[b] SwRI	[c] NRL
83-57	56.6	3.2	-1.7	-0.8	-2.5	3.7	3.8
83-8	56.5	1.2	-4.6	-3.6	-4.4	-3.1	-2.2
83-15	55.2	5.6	-2.6	-1.7	-2.7	3.9	5.3
83-68	54.6	-0.6	-1.1	1.1	-0.5	2.6	3.5
83-30	54.6	4.7	-0.6	0.9	-0.6	-2.6	-1.9
83-19	54.5	0.0	-3.8	-2.2	-2.9	0.3	2.0
83-72	53.8	-1.5	-0.2	4.0	1.7	4.7	5.2
83-14	52.9	0.7	-2.2	-0.6	-1.3	0.4	0.9
83-71	52.5	1.1	-4.0	-2.0	-2.3	0.6	1.1
83-69	52.4	1.8	-1.6	0.3	-0.5	-1.3	-0.5
83-78	52.1	1.4	2.4	5.1	3.1	5.9	5.8
83-20	52.0	1.7	-2.3	-0.9	-1.3	3.5	4.0
83-25	51.3	4.4	-1.8	-0.7	-1.0	1.0	1.7
83-17	50.4	3.1	-0.8	0.8	0.3	0.2	0.9
83-31	50.0	6.7	-0.9	0.0	-0.2	2.6	2.2
83-22	49.9	0.0	-1.6	0.1	0.1	0.4	0.9
83-12	49.8	4.5	-0.6	0.8	0.7	-0.8	0.4
83-80	48.7	5.1	-0.6	0.3	0.3	-1.6	-0.6
83-26	48.7	0.4	0.9	2.0	1.7	3.4	3.9
83-27	48.5	3.9	2.1	4.1	3.3	1.2	2.1
83-81	47.8	1.9	-0.2	1.7	1.6	-1.9	-0.8
83-7	47.7	5.9	-1.7	-0.7	-0.3	0.4	2.2
83-24	47.3	12.2	1.6	2.3	2.2	2.9	2.9
83-78	47.1	3.3	3.2	6.2	5.3	-0.4	0.8
83-10	46.8	-7.8	-7.5	-5.6	-4.6	-14.3	-13.4
83-16	45.7	-4.5	-3.9	-2.3	-1.5	3.2	4.2
83-23	45.6	-0.2	-2.0	-0.6	0.3	4.8	6.0
83-13	45.8	-5.8	-2.8	-0.5	0.4	4.6	4.3
83-11	40.9	-2.3	-2.1	-0.1	0.9	-7.2	-6.3
83-9	54.3	ND	ND	ND	ND	3.3	3.4
83-37	50.2	ND	ND	ND	ND	2.1	2.9
83-74	48.6	-0.6	ND	-0.8	-2.6	1.1	2.4
83-35	47.8	ND	ND	ND	ND	-2.1	-1.0

[a] Formulations of these cetane indices are given in Appendix B1.2 - B2

[b] Based on integrations performed at SwRI

[c] Based on integrations performed at NRL using SwRI's FIDs.

Table 7

Evaluation of a Trial Cetane Index Based on Refractive Index and Density
(Worldwide Survey I of Commercial Marine Fuels)

NRL ID	CETANE NO. (ASTM D613)	DENSITY	REFRACTIVE INDEX (@ 25 deg C)	CETANE INDEX 2 2 (D ,RI , RI/D) *	DIFFERENCE CI - CN **
83-67	56.6	0.8443	1 4714	52.3	-4.3
83-8	56.5	0.8433	1.4688	52.4	-4.1
83-15	55.2	0.8358	1.4666	51.0	-4.2
83-68	54.6	0.8623	1.4801	49.7	-4.9
83-30	54.6	0.8453	1.4705	52.4	-2.2
83-19	54.5	0.8524	1.4744	52.0	-2.5
83-14	52.9	0.8555	1.4754	51.5	-1.4
83-71	52.5	0.8509	1.4755	52.2	-0.3
83-69	52.4	0.8545	1.4747	51.7	-0.7
83-76	52.1	0.8670	1.4831	47.8	-4.3
83-20	52.0	0.8519	1.4778	52.2	0.2
83-35	51.3	0.8443	1.4696	52.4	1.1
83-17	50.4	0.8529	1.4732	51.9	1.5
83-31	50.3	0.8393	1.4656	52.0	1.7
83-22	48.8	0.8628	1.4809	49.6	0.8
83-12	48.8	0.8493	1.4721	52.3	3.5
83-36	48.7	0.8665	1.4819	48.0	-0.7
83-80	48.7	0.8458	1.4698	52.5	3.8
83-27	48.5	0.8602	1.4797	50.4	1.9
83-81	47.8	0.8612	1.4782	49.9	2.1
83-7	47.7	0.8409	1.4662	52.2	4.5
83-34	47.3	0.8289	1.4596	49.2	1.9
83-78	47.1	0.8686	1.4799	46.5	-0.6
83-10	46.8	0.8762	1.4809	41.5	-5.3
83-16	45.7	0.8745	1.4991	46.4	0.7
83-23	43.6	0.8644	1.4855	49.4	5.8
83-11	40.9	0.8742	1.4811	41.6	0.7
83-9	54.3	0.8565	Dark	ND	ND
83-72	53.8	0.8718	Dark	ND	ND
83-37	50.2	0.8629	Dark	ND	ND
83-74	48.6	0.8724	1.4846	44.9	-3.7
83-26	47.8	0.8670	Too dark	ND	ND
83-24	42.8	0.8883	Dark	ND	ND

* $CI = 7200.3 - 4972.2\ D + 1641.04(RI)^2 - (4106.72 * RI/D)^2$

** Cetane Index - Cetane Number

Table 8: Determination of the Frequency of Predictability of Cetane Indices

A: Published Cetane Indices That Are Based on Density and Distillation Temperatures
(Worldwide Survey I Commercial Marine Fuels)

	Frequency of Predictability For Specific Predictive Ranges: For 28 Fuels				
PREDICTIVE RANGE (CI - CN)*	CCI ASTM D976-66	CCI ASTM D976-80	INGHAM'S DISTN. TEMP. DENSITY EQN	IMPROVEMENT EQUATIONS OF D976-80 ETHYL EQN	COLLINS**
Predictions Within:					
0 - 1.0	5	4	8	5	4
-(0.1 - 1.0)	1	5	4	6	7
1.1 - 2.0	5	3	3	3	6
-(1.1 - 2.0)	0	7	5	1	0
Underpredictions Within:					
-(2.1 - 3.0)	3	6	2	1	2
-(3.1 - 4.0)	0	1	1	1	2
-(4.1 - 5.0)	0	1	0	2	1
-(> 5.0)	0	0	0	0	0
Overpredictions Within:					
2.1 - 3.0	8	0	2	6	3
3.1 - 4.0	0	1	1	1	2
4.1 - 5.0	3	0	2	1	0
> 5.0	3	0	0	1	1

* Cetane Index - Cetane Number

** Collins and Unzelman Equation

Table 8: Determination of the Frequency of Predictability of Cetane Indices

A: Published Cetane Indices That Are Based on Density and Distillation Temperatures
(Worldwide Survey I Commercial Marine Fuels)

	Frequency of Predictability For Specific Predictive Ranges: For 78 Fuels				
PREDICTIVE RANGE (CI - CN)*	CCI ASTM D976-66	CCI ASTM D976-80	INGHAM'S DISTN. TEMP. DENSITY EQN	IMPROVEMENT EQUATIONS OF D976-80 ETHYL EQN	COLLINS**
Predictions Within:					
0 - 1.0	5	4	8	5	4
-(0.1 - 1.0)	1	5	4	6	7
1.1 - 2.0	5	3	3	3	6
-(1.1 - 2.0)	0	7	5	1	0
Underpredictions Within:					
-(2.1 - 3.0)	3	6	2	1	2
-(3.1 - 4.0)	0	1	1	1	2
-(4.1 - 5.0)	0	1	0	2	1
-(> 5.0)	0	0	0	0	0
Overpredictions Within:					
2.1 - 3.0	8	0	2	6	3
3.1 - 4.0	0	1	1	1	2
4.1 - 5.0	3	0	2	1	0
> 5.0	3	0	0	1	1

* Cetane Index - Cetane Number

** Collins and Uzelac Equation

Table 8: Determination of the Frequency of Predictability of Cetane Indices

8: Includes Three Trial Cetane Indices That Are Based on Density and Distillation Temperatures
(Worldwide Survey I Commercial Marine Fuels)

	Frequency of Predictability For Specific Predictive Ranges: For 28 Fuels			
		Trial Cetane Indices		
PREDICTIVE RANGE (CI - CN)*	CCI ASTM D976-80	Modified ASTM D976-80 AVG(MBP)**	LOTUS 1-2-3 REGRESSION ANALYSIS T50, D	AVG(MBP)**
Predictions Within:				
0 - 1.0	4	2	5	4
-(0.1 - 1.0)	5	7	5	7
1.1 - 2.0	3	6	4	5
-(1.1 - 2.0)	7	7	6	4
Underpredictions Within:				
-(2.1 - 3.0)	6	3	3	2
-(3.1 - 4.0)	1	0	0	1
-(4.1 - 5.0)	1	1	1	1
-(> 5.0)	0	0	0	0
Overpredictions Within:				
2.1 - 3.0	0	1	3	3
3.1 - 4.0	1	1	0	1
4.1 - 5.0	0	0	1	0
> 5.0	0	0	0	0

* Cetane Index - Cetane Number

** AVG.(MBP) = AVG.(T10, T50, T90), deg C

Table 8: Determination of the Frequency of Predictability of Cetane Indices

C: Cetane Indices That Are Based on Various Types of Parameters
(Worldwide Survey I Commercial Marine Fuels)

PREDICTIVE RANGE (CI - CN)*	Frequency of Predictability For Specific Predictive Ranges: For 28 Fuels **						
	DIESEL INDEX (G, API)	CGSB EQUATION (T,D,API,VISC)	INGHAM'S ANILINE PT EQN (API)	TRIAL ANILINE PT. EQN (API)	SwRI CETANE INDEX (PROTON NMR ANALYSIS) SwRI	NRL	TRIAL RI/D *** CET. INDEX FOR 26 FUELS
Predictions Within:							
0 - 1.0	4	1	7	7	7	5	4
-(0.1 - 1.0)	2	7	8	6	2	3	4
1.1 - 2.0	6	1	3	3	1	2	5
-(1.1 - 2.0)	1	7	2	3	3	1	1
Underpredictions Within:							
-(2.1 - 3.0)	1	5	2	4	1	1	2
-(3.1 - 4.0)	0	3	1	0	1	0	0
-(4.1 - 5.0)	1	1	0	1	0	0	5
-(> 5.0)	1	0	0	0	1	1	0
Overpredictions Within:							
2.1 - 3.0	0	2	1	1	3	5	1
3.1 - 4.0	4	1	1	2	5	4	2
4.1 - 5.0	3	0	1	0	3	2	1
> 5.0	5	0	2	1	1	4	1

* Cetane Index - Cetane Number

** Unless otherwise stated

*** Trial cetane index based on refractive index and density (see Table 7)

Table 9: Determination of the % Predictability of Cetane Indices

A: Published Cetane Indices That Are Based on Density and Distillation Temperatures
(Worldwide Survey I Commercial Marine Fuels)

	% Predictability For Specific Predictive Ranges: For 28 Fuels				
PREDICTIVE RANGE (CI - CN)*	CCI ASTM D976-66	CCI ASTM D976-80	INGHAM'S DISTN. TEMP. DENSITY EQN	IMPROVEMENT EQUATIONS OF D976-80 ETHYL EQN	COLLINS**
Predictions Within:					
0 - 1.0	17.9	14.3	28.6	17.9	14.3
-(0.1 - 1.0)	3.6	17.9	14.3	21.4	25.0
1.1 - 2.0	17.9	10.7	10.7	10.7	21.4
-(1.1 - 2.0)	0.0	25.0	17.9	3.6	0.0
Total: +/- (0 - 2.0)	39.3	67.9	71.4	53.6	60.7
Underpredictions Within:					
-(2.1 - 3.0)	10.7	21.4	7.1	3.6	7.1
-(3.1 - 4.0)	0.0	3.6	3.6	3.6	7.1
-(4.1 - 5.0)	0.0	3.6	0.0	7.1	3.6
-(> 5.0)	0.0	0.0	0.0	0.0	0.0
Total: -(2.1 - >5.0)	10.7	28.6	10.7	14.3	17.9
Overpredictions Within:					
2.1 - 3.0	28.6	0.0	7.1	21.4	10.7
3.1 - 4.0	0.0	3.6	3.6	3.6	7.1
4.1 - 5.0	10.7	0.0	7.1	3.6	0.0
> 5.0	10.7	0.0	0.0	3.6	3.6
Total: (2.1 - >5.0)	50.0	3.6	17.9	32.1	21.4

* Cetane Index - Cetane Number

** Collins and Unzelman Equation

Table 9: Determination of the % Predictability of Cetane Indices

B: Includes Three Trial Cetane Indices That Are Based on Density and Distillation Temperatures
(Worldwide Survey I Commercial Marine Fuels)

	% Predictability For Specific Predictive Ranges: For 28 Fuels			
		Trial Cetane Indices		
PREDICTIVE RANGE (CI - CN)*	CCI ASTM D976-80	Modified ASTM D976-80 AV(MBP)**	LOTUS 1-2-3 REGRESSION ANALYSIS T50, D	AVG(MBP)**
Predictions Within:				
0 - 1.0	14.3	7.1	17.9	14.3
-(0.1 - 1.0)	17.9	25.0	17.9	25.0
1.1 - 2.0	10.7	21.4	14.3	17.9
-(1.1 - 2.0)	25.0	25.0	21.4	14.3
Total: +/-(0 - 2.0)	67.9	78.6	71.4	71.4
Underpredictions Within:				
-(2.1 - 3.0)	21.4	10.7	10.7	7.1
-(3.1 - 4.0)	3.6	0.0	0.0	3.6
-(4.1 - 5.0)	3.6	3.6	3.6	3.6
-(> 5.0)	0.0	0.0	0.0	0.0
Total: -(2.1 - >5.0)	28.6	14.3	14.3	14.3
Overpredictions Within:				
2.1 - 3.0	0.0	3.6	10.7	10.7
3.1 - 4.0	3.6	3.6	0.0	3.6
4.1 - 5.0	0.0	0.0	3.6	0.0
> 5.0	0.0	0.0	0.0	0.0
Total: (2.1 - >5.0)	3.6	7.1	14.3	14.3

* Cetane Index - Cetane Number

** AVG.(MBP) = AVG.(T10, T50, T90), deg C

Table 9: Determination of the % Predictability of Cetane Indices

C: Cetane Indices That Are Based on Various Types of Parameters
(Worldwide Survey I Commercial Marine Fuels)

PREDICTIVE RANGE (CI - CN)	% Predictability For Specific Predictive Ranges: For 28 Fuels *						
	DIESEL INDEX (G, API)	CCSB EQUATION (T,D,API,VISC)	INGHAM'S ANILINE PT EQN (API)	TRIAL ANILINE PT. EQN (API)	SwRI CETANE INDEX (PROTON NMR ANALYSIS) SwRI	NRL	TRIAL RI/D CETANE INDEX ** FOR 26 FUELS
Predictions Within:							
0 - 1.0	14.3	3.6	25.0	25.0	25.0	17.9	15.4
-(0.1 - 1.0)	7.1	25.0	28.6	21.4	7.1	10.7	15.4
1.1 - 2.0	21.4	3.6	10.7	10.7	3.6	7.1	19.2
-(1.1 - 2.0)	3.6	25.0	7.1	10.7	10.7	3.6	3.8
Total: +/- (0 - 2.0)	46.4	57.1	71.4	67.9	46.4	39.3	53.8
Underpredictions Within:							
-(2.1 - 3.0)	3.6	17.9	7.1	14.3	3.6	3.6	7.7
-(3.1 - 4.0)	0.0	10.7	3.6	0.0	3.6	0.0	0.0
-(4.1 - 5.0)	3.6	3.6	0.0	3.6	0.0	0.0	19.2
-(> 5.0)	3.6	0.0	0.0	0.0	3.6	3.6	0.0
Total: -(2.1 - >5.0)	10.7	32.1	10.7	17.9	10.7	7.1	26.9
Overpredictions Within:							
2.1 - 3.0	0.0	7.1	3.6	3.6	10.7	17.9	3.8
3.1 - 4.0	14.3	3.6	3.6	7.1	17.9	14.3	7.7
4.1 - 5.0	10.7	0.0	3.6	0.0	10.7	7.1	3.8
> 5.0	17.9	0.0	7.1	3.6	3.6	14.3	3.8
Total: (2.1 - >5.0)	42.9	10.7	17.9	14.3	42.9	53.6	19.2

* Unless otherwise stated

** Trial cetane index for refractive index and density (see Table 7)

Table 10

Measure of Predictability of Various Cetane Indices
(Worldwide Survey I Commercial Marine Fuels)

Cetane Index	Parameters	Predictability For a 28 Fuel Set[a]		
		% Predicted	% Over-Predicted	% Under-Predicted
ASTM D 976-80 (Modified)	AVG.(T10,T50,T90), Density	78.6	7.1	14.3
Trial	AVG.(T10,T50,T90), Density	71.4	14.3	14.3
Trial	T50, Density	71.4	14.3	14.3
Ingham's Distilln Temps / Density Eqn	T10,T50,T90, Density	71.4	17.9	10.7
Ingham's Aniline Point Eqn	Aniline Point	71.4	17.9	10.7
ASTM D 976-80	T50, Density	67.9	3.6	28.6
Trial	Aniline Point	67.9	14.3	17.9
Collins and Umzelman Eqn[b]	T50, Density	60.7	21.4	17.9
Canadian General Standards Board	T10,T50,T90, Density Aniline Point, Viscosity	57.1	10.7	32.1
Ethyl Equation[b]	T50, Density	53.6	32.1	14.3
Southwest Research Inst.[c]	Proton type,Density,% Hydrogen	46.4	42.9	10.7
Diesel Index	API Gravity, Aniline Point	46.4	42.9	10.7
ASTM D 976-66	T50, API Gravity	39.3	50.0	10.7
Southwest Research Inst.[d]	Proton type,Density,% Hydrogen	39.3	53.6	7.1
Trial[e]	Refractive Index, Density	53.8	19.2	26.9

Footnotes for Table 10

where:

a
Unless otherwise stated; 28 Fuel set includes 17 MGOs, 7 HMGOs, and 4MOFs.

b
Improvement Equation of D976-80 (see Appendix B1.1.1, No.3)

c
Proton NMR analyses including integrations performed at Southwest Research Institute (SwRI)

d
Integrations performed at NRL using SwRI's Free Induction Decay Data

e
For 26 of the 28 fuel set mentioned in a, above

Table II

Regression Analyses of Cetane Number Vs Cetane Index For Various Cetane Indices
(Worldwide Survey I Commercial Marine Fuels)

Cetane Index	Parameters	R^2 Values For:	
		[a] 28 Fuels	[b] 28+44 Fuels
Ingham's Distn.Temp. / Density Eqn	T10,T50,T90 , Density	0.817	0.756
Collins and Unzelman Eqn [c]	T50, Density	0.809	0.744
Ethyl Equation [c]	T50, Density	0.806	0.735
ASTM D 976-80 (Modified)	AVG.(T10,T50,T90), Density	0.800	0.730
ASTM D 976-80	T50, Density	0.799	0.721
Canadian General Standards Board	T10,T50,T90, Density Aniline Point, Viscosity	0.797	0.759
Trial	AVG.(T10,T50,T90), Density	0.779	0.719
ASTM D 976-66	T50, API Gravity	0.776	0.711
Trial	T50, Density	0.765	0.703
Trial	Aniline Point	0.737	0.705
Ingham's Aniline Point Eqn	Aniline Point	0.727	0.703
Southwest Research Inst. [d]	Proton type,Density,% Hydrogen	0.720	0.612
Southwest Research Inst. [e]	Proton type,Density,% Hydrogen	0.700	0.597
Diesel Index	API Gravity, Aniline Point	0.657	0.638
Trial	Refractive Index, Density	0.448 [f]	0.417 [g]

Footnotes for Table II

where:

*A refers to M80 87-10. The cetane no., of this fuel was much higher than most of the cetane indices evaluated.

a

28 Fuel set includes 17 M60s, 7 HM60s, and 4MDFs.

b

28 Fuel set includes the same as 'a' above plus A*.

c

Improvement Equation of D976-80

d

Integrations performed at NRL using SwRI's Free Induction Decay Data.

e

Proton NMR analyses including integrations performed at Southwest Research Institute (SwRI).

f

For 25 of the 28 fuel set referred to in 'a' above .

g

For 27 fuels and includes the 25 fuel set in 'f' above plus A*.

Table 12

Cetane Index Vs Cetane Number: Regression Analysis and Measure of Predictability
(Worldwide Survey I Comaercial Marine Fuels)

Cetane Index	Parameters	R^2 Values For:	Measure of % Predictability For 28 Fuels *		
		28 Fuels *	Predict	Over-Predict	Under-Predict
Ingnam's Distn.Temp. / Density Eqn	T10,T50,T90 , Density	0.817	71.4	17.9	10.7
Collins and Unzelwar Eqn	T50, Density	0.809	60.7	21.4	17.9
Ethyl Equation	T50, Density	0.806	53.6	32.1	14.3
ASTM D 976-80 (Modified)	AVG.(T10,T50,T90), Density	0.800	78.6	7.1	14.3
ASTM D 976-80	T50, Density	0.799	67.9	3.6	28.6
Canadian General Standards Board	T10,T50,T90, Density Aniline Point, Viscosity	0.797	57.1	10.7	32.1
Trial	AVG.(T10,T50,T90), Density	0.779	71.4	14.3	14.3
ASTM D 976-66	T50, API Gravity	0.776	39.3	50.0	10.7
Trial	T50, Density	0.765	71.4	14.3	14.3
Trial	Aniline Point	0.737	67.9	14.3	17.9
Ingham's Aniline Point Eqn	Aniline Point	0.727	71.4	17.9	10.7
Southwest Research Inst. (NRL)**	Proton type,Density,% Hydrogen	0.720	39.3	53.6	7.1
Southwest Research Inst. (SwRI)	Proton type,Density,% Hydrogen	0.700	46.4	42.9	10.7
Diesel Index	API Gravity, Aniline Point	0.657	46.4	42.9	10.7
Trial (For 26 of the 28 Fuels)	Refractive Index, Density	0.448	53.8	19.2	26.9

* Unless otherwise stated

** Integrations performed at NRL using SwRI Free Induction Decay data

*** Proton NMR analyses including integrations performed at SwRI

Figure 1

Predictability of Modified ASTM D976-80

For 28 Fuels

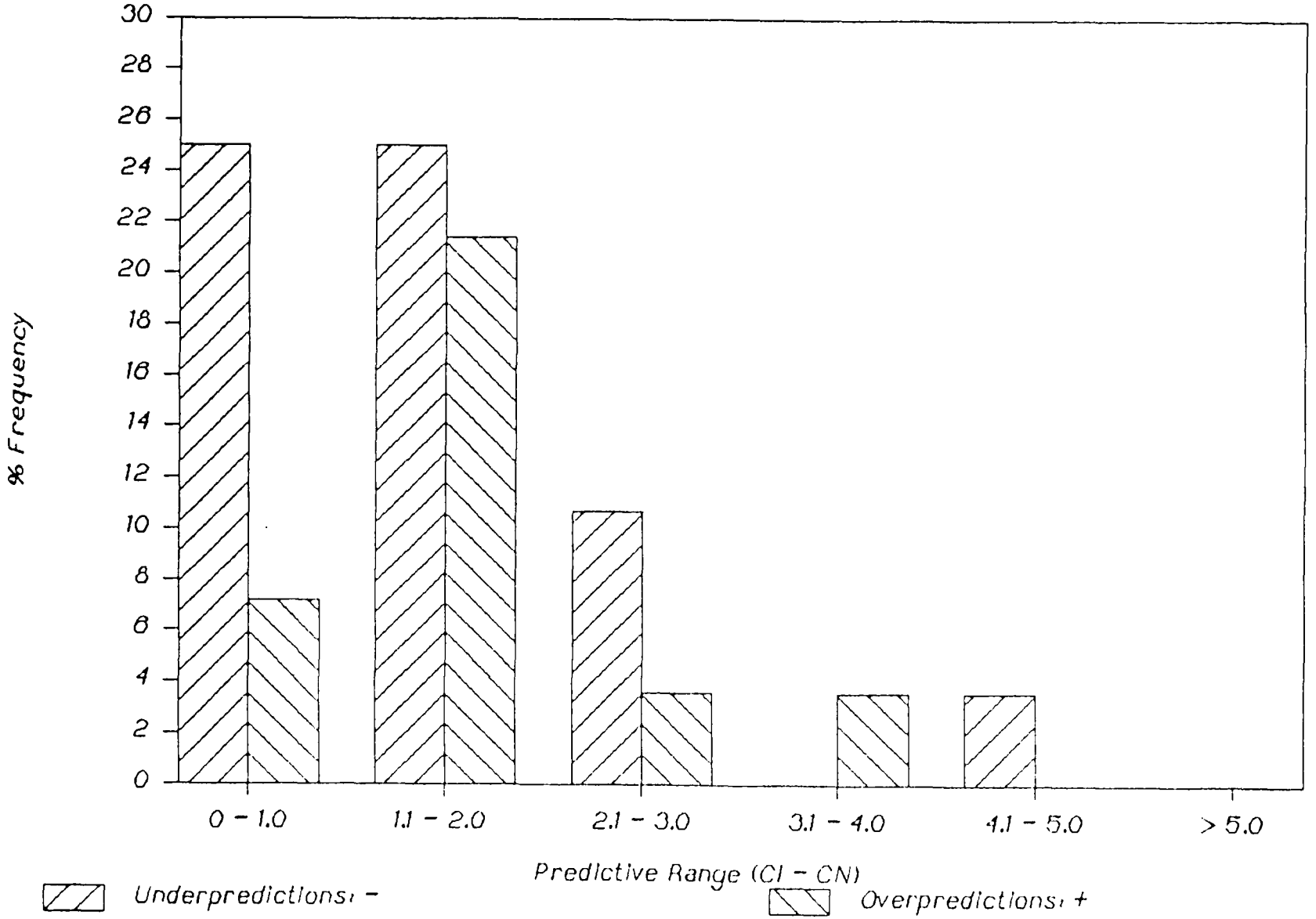


Figure 2

Predictability of Ingham's Cetane Index

Eqn For 28 Fuels

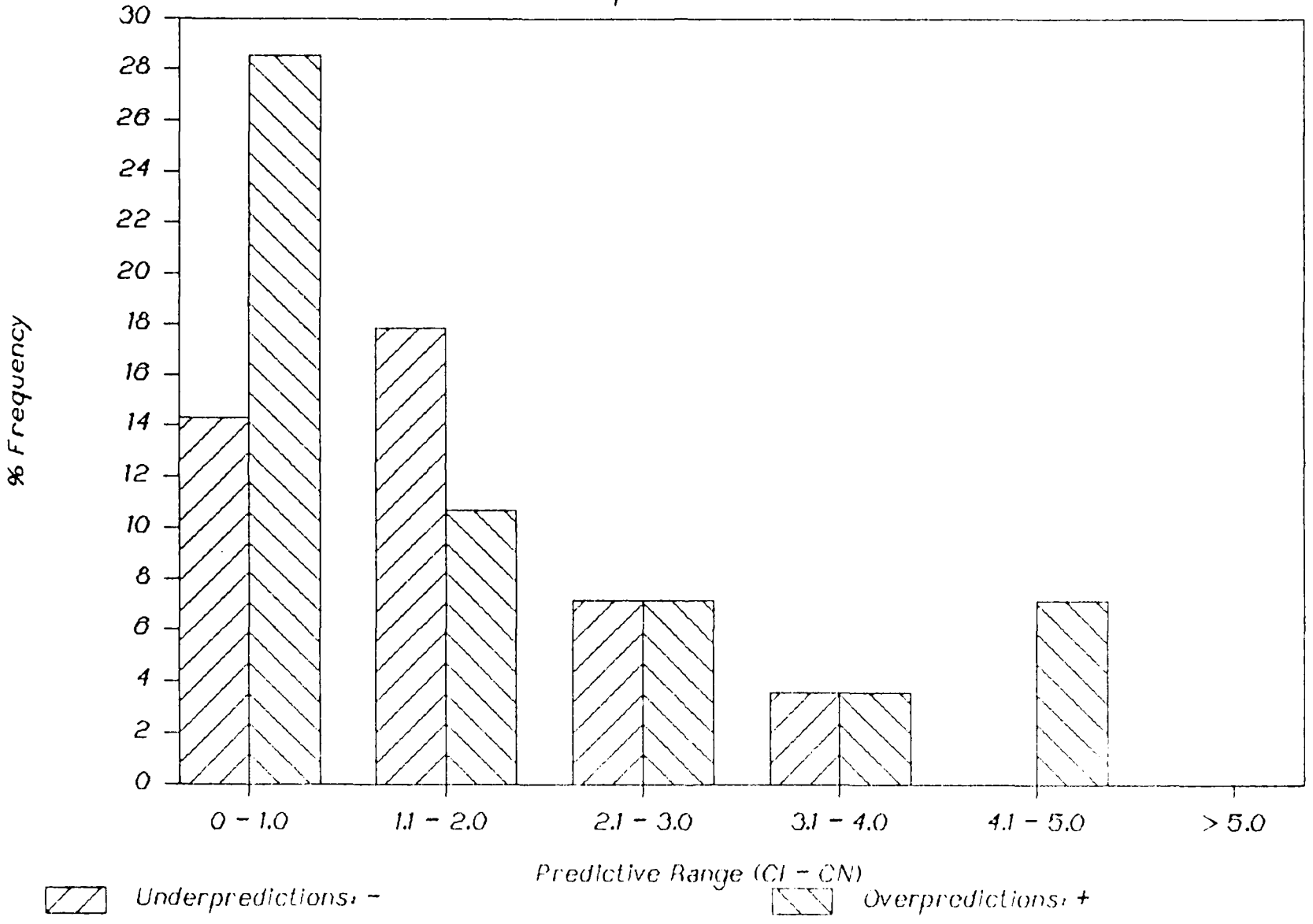


Figure 3

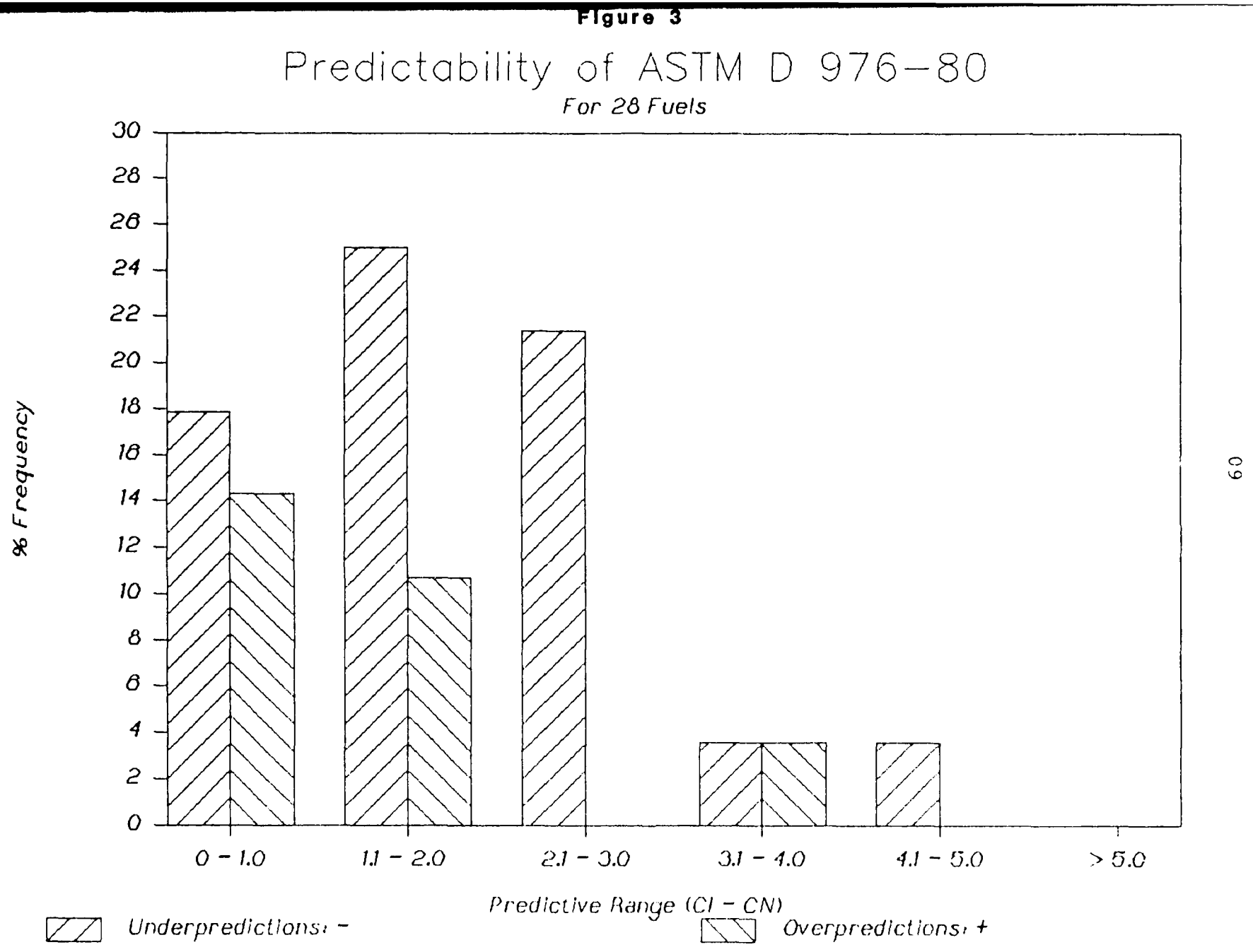

Predictability of ASTM D 976-80
For 28 Fuels
% Frequency
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
0 - 1.0
1.1 - 2.0
2.1 - 3.0
3.1 - 4.0
4.1 - 5.0
> 5.0
Predictive Range (CI - CN)
Underpredictions: -
Overpredictions: +

Figure 4

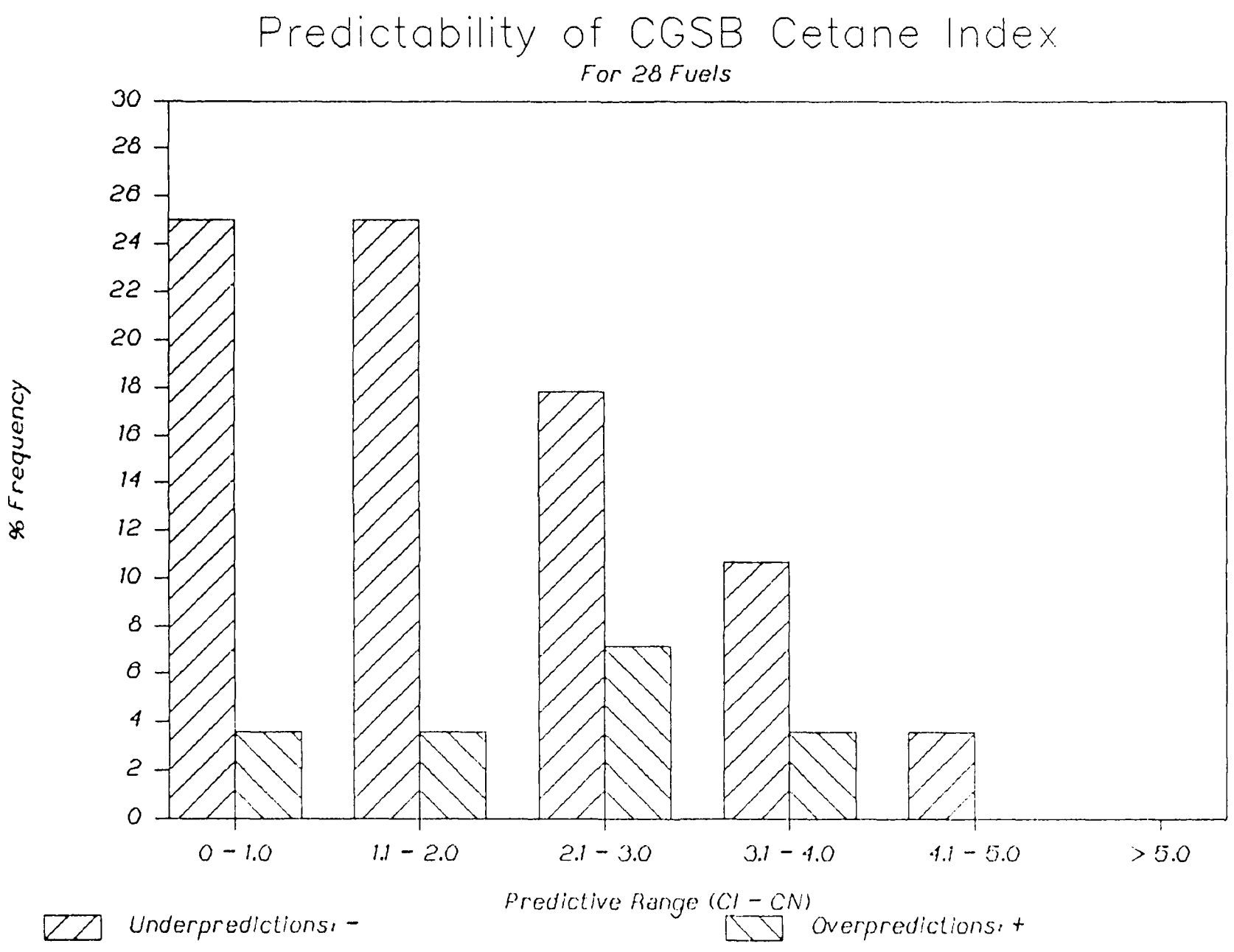
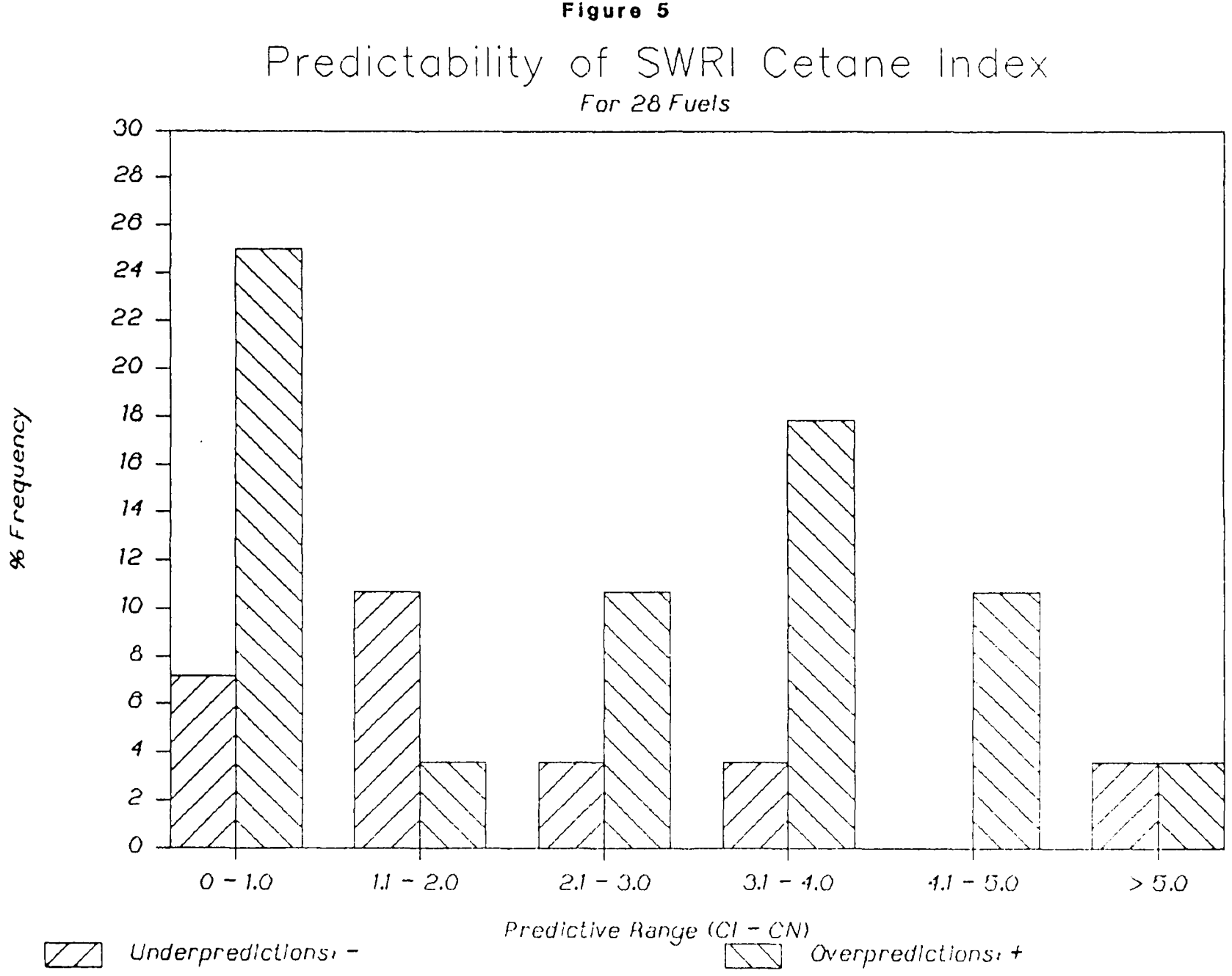

Predictability of CGSB Cetane Index
For 28 Fuels
% Frequency
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
0 - 1.0
1.1 - 2.0
2.1 - 3.0
3.1 - 4.0
4.1 - 5.0
> 5.0
Predictive Range (CI - CN)
Underpredictions: -
Overpredictions: +

Figure 5


Predictability of SWRI Cetane Index
For 28 Fuels
% Frequency
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
0 - 1.0
1.1 - 2.0
2.1 - 3.0
3.1 - 4.0
4.1 - 5.0
> 5.0
Predictive Range (CI - CN)
Underpredictions -
Overpredictions +

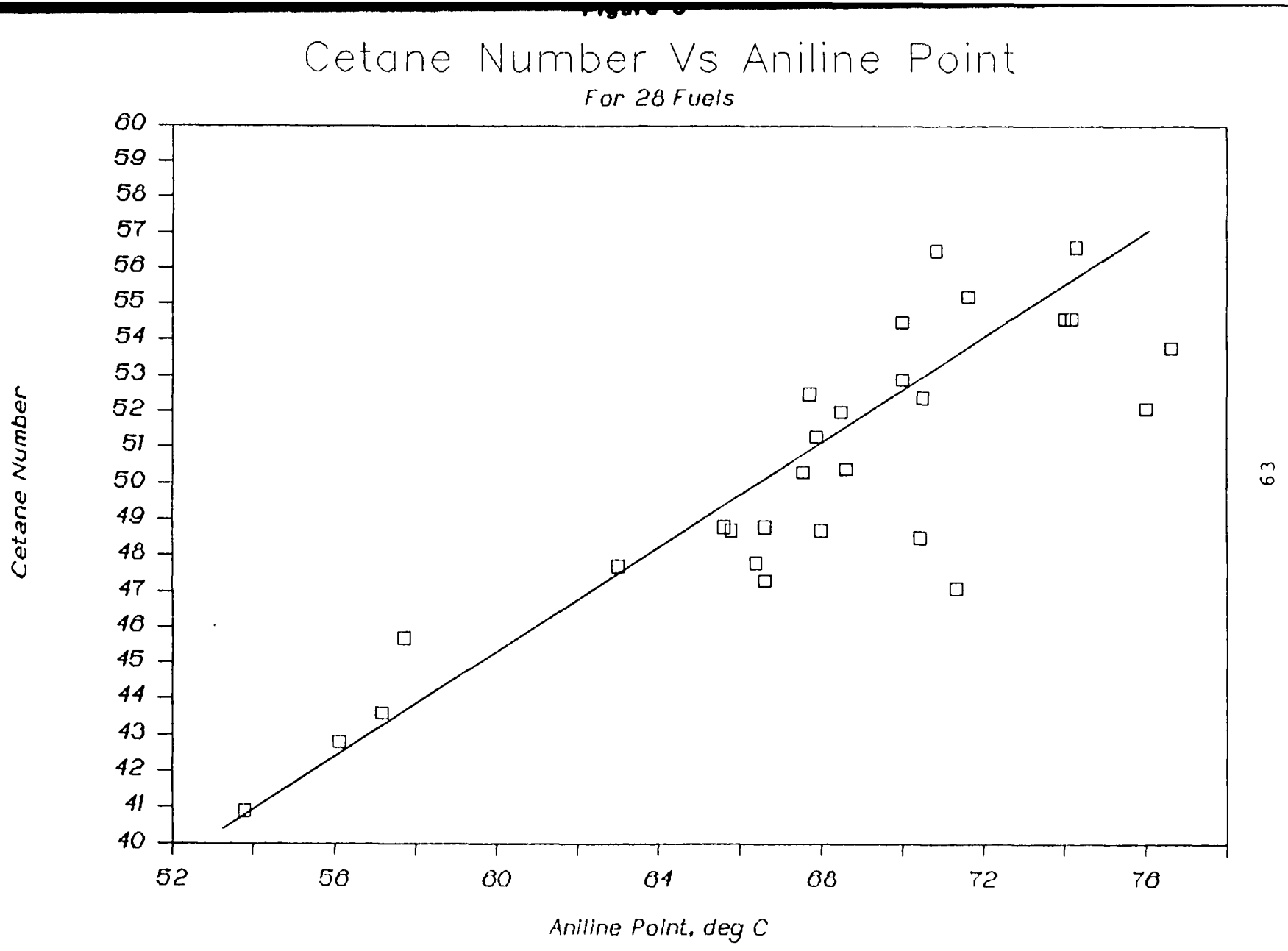
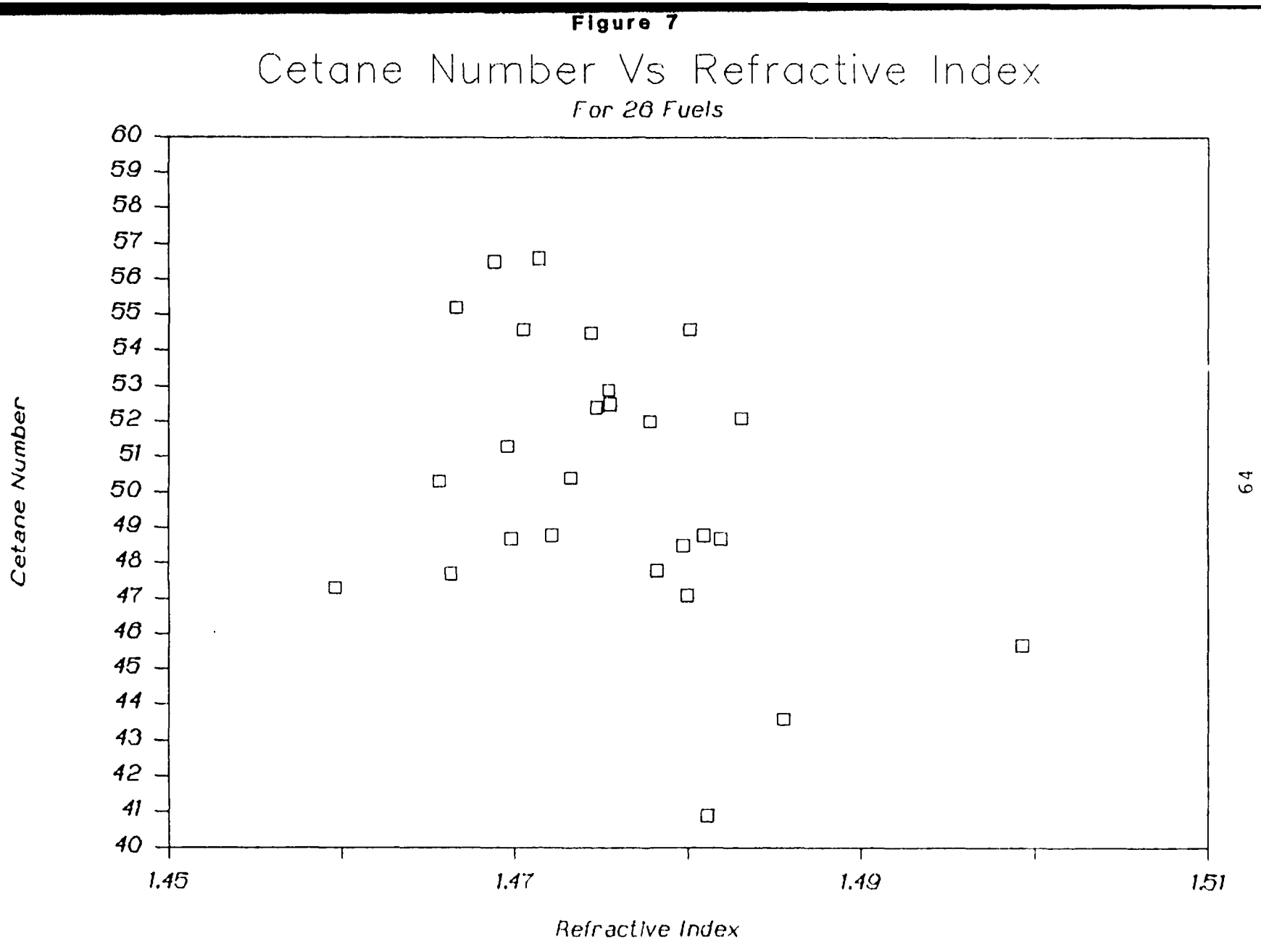

Cetane Number Vs Aniline Point
For 28 Fuels
Cetane Number
60
59
58
57
56
55
54
53
52
51
50
49
48
47
46
45
44
43
42
41
40
52
56
60
64
68
72
76
Aniline Point, deg C

Figure 7


Cetane Number Vs Refractive Index
For 26 Fuels
Cetane Number
60
59
58
57
56
55
54
53
52
51
50
49
48
47
46
45
44
43
42
41
40
1.45
1.47
1.49
1.51
Refractive Index
64

APPENDIX A

List of Symbols

(Symbols listed pertain to those parameters employed in the formulations of the cetane indices given in Appendix B).

AP	Aniline Point in deg C or deg F, as specified (ASTM D611).
CI	Cetane Index.
CCI	Calculated Cetane Index (ASTM D976).
D	Density at 15 deg C, g/mL (ASTM D1298).
G	API Gravity, deg API (ASTM D287 or D1298).
H	Hydrogen content, wt% (ASTM D3701).
M	50% Distillation temperature *, deg F, (ASTM D86).
PCN	Predicted Cetane Number.
T10	10% Distillation temperature *, deg C (ASTM D86).
T50	50% Distillation temperature *, deg C (ASTM D86).
T90	90% Distillation temperature *, deg C (ASTM D86).
Visc	Viscosity: at 40 deg C, cSt, (ASTM D445).

* % Distillation Temperature refers to the distillation temperature of % recovered distillate.

APPENDIX B: Cetane Indices Formulations

B1 CETANE INDICES BASED ON PHYSICAL PROPERTIES

B1.1 Indices Which Employ Distillation Temperature(s) and Density

B1.1.1 Published Cetane Indices

1. Calculated Cetane Index (CCI)

a) ASTM D976-66 [2a]

$$CCI = 0.49083 + 1.06577\ X - 0.0010552\ X^2$$

where:

$$X = 97.833 \log M^2 + 2.2088\ G \log M + 0.01247\ G^2 - 423.51 \log M - 4.7808\ G + 419.59$$

G = API gravity in deg API.

M = Distillation temperature in deg F of 50% recovered distillate.

b) ASTM D976-80 [2b]

$$CCI = 454.74 - 1641.416\ D + 774.74\ D^2 - 0.554\ T50 + 97.803\ (\log T50)^2$$

where:

D = Density at 15 deg C, g/mL.

T50 = Distillation temperature in deg C of 50% recovered distillate.

Note: Conversion of API Gravity to Density were made using the relationship given in ASTM D287 [7], which is:

G = (141.5/sp gr 60/60 F) - 131.5
where density was substituted for specific gravity

2. **Ingham et al.'s Four Variable Equation: Proposed Replacement Equation for D976-80 [10]**

$$PCN = 45.2 + 0.0892*T10N + (0.131 + 0.901*B)*T50N + (0.0523 - 0.420*B)*T90N + 4.90E-4*(T10N^2 - T90N^2) + 107*B + 60.0*B^2$$

where:
PCN = Predicted Cetane Number
B = EXP(-3.50 * DN) - 1
DN = (D - 0.850)
T10N = (T10N - 215)
T50N = (T50 - 260)
T90N = (T90 - 310)

T10, T50, T90 refer to the distillation temperatures in deg C of 10, 50, and 90% recovered distillate, respectively.

Note: The suffix, N, of the physical properties parameters refer to normalization.

3. **Improvement Equations of ASTM D976-80**

a) Collins and Unzelman Equation [3]

$$PCN = 21.843 - 0.33924\ (CCI) + 0.018669\ (CCI)^2$$

b) Ethyl Equation [11]

$$PCN = 5.28 + 0.371\ (CCI) + 0.0112\ (CCI)^2$$

B1.1.2 Trial Cetane Indices Based on Regression Analysis of 28 Fuels Evaluated in This Study

1. **Index Based on Mid-boiling Point and Density**

$$CI = 243.7838 + 0.1640\ T50 - 281.401\ D$$

2. **Index Based on Average Mid-boiling Point and Density**

$$CI = 254.0107 + 0.1724\ T50_{AV} - 296.882\ D$$

where: $T50_{AV}$ = Average (T10+T50+T90), deg C

B1.2 Index Which Employs Distillation Temperatures, Density, Aniline Point, and Viscosity

Canadian General Standards Board Cetane Index (CGSB) [12]

$$CI = 77.7628 + 0.1765\ AP + 0.003867\ AP^2 - 11.6150\ Kc + 0.5844\ Kc^2 - 0.6350\ Visc$$

where:

CI = Cetane Index

AP = Aniline Point, deg C

$$Kc = \frac{T10 + T50 + T90 + 820}{200 * D^2}$$

Visc = Viscosity at 40 deg C in cSt

B1.3 Indices Which Employ Aniline Point Only

B1.3.1 Published Cetane Index

Ingham et al's Aniline Point Equation [10]

$$PCN = -0.611 + 45.5*EXP(0.0150*APN)$$

where: APN = (AP - 60); the suffix, N, refers to normalization; and aniline point is in deg C

B1.3.2 Trial Cetane Index Based on Regression Analysis of 28 Fuels Evaluated in This Study

$$CI = 9.48854 + 0.601223\ AP$$

where AP is in deg C

B1.4 Index Which Employs Aniline Point and API Gravity

$$\text{Diesel Index} = \frac{G * AP}{100} \qquad [5]$$

where AP is in deg F

B1.5 Trial Cetane Index Which Employs Refractive Index and Density

$$CI = 7200.8 - 4972.20\ D^2 + 1641.04\ (RI)^2 - (4106.72 * RI/D)$$

where: RI is the refractive index measured at 25.1 deg C.

B2 CETANE INDEX BASED ON PROTON NMR COMPOSITIONAL ANALYSIS

Southwest Research Institute Cetane Index (SwRI) [9]

$$PCN = 9.49 - 0.0298(D * H * H_{CH3}) + 0.0896(D * H * H_{CH2}) + 0.000097(D * H * S^2) - 0.038(D * H * H_{ALPHA})$$

where:

H	=	wt% Hydrogen content
H_{CH3}	=	% Methyl proton of total number of protons
H_{CH2}	=	% Methylene protons of total number of protons
S	=	Sum of % (methyl, methylene, and methine) protons
H_{ALPHA}	=	% Alpha protons (protons immediately adjacent to an aromatic ring).

APPENDIX C

Proton Chemical Shift Assignment *

Proton Type	Chemical Shift (ppm, delta)
Alkane Methyl	0.5 - 1.05
Gamma Methyl	0.5 - 1.05
Alkane Methylene	1.05 - 1.4
Beta Methyl	1.05 - 1.4
Gamma Methylene	1.05 - 1.4
Alkane Methine	1.4 - 2.0
Cycloalkane Methylene	1.4 - 2.0
Beta Methylene	1.4 - 2.0
Alpha Methyl	2.0 - 4.4
Alpha Methylene	2.0 - 4.4
Alpha Methine	2.0 - 4.4
Aromatics	6.2 - 9.2

* Bailey et al [9]

APPENDIX D1

Method of Converting Fractions of Total Carbon Data Derived From HPLC Analysis to % Based on Weight

1. Fraction of total carbon for a specific class of compound was converted to its fractional weight using the following formula:

   Fractional Weight of Compound Class =
   Fraction Total Carbon * [1 + (No. H atoms/Molecular Wt. of Compound Class)]

2. % Fractional Weight was obtained by normalizing the fractional weight of the various classes of compounds to 100

APPENDIX D2

Compositional Analysis of Worldwide Survey I Commercial Marine Fuels

Differences Between Measured and Calculated Values For Saturates and Monocyclic Aromatics *

	SATURATES				MONOCYCLIC AROMATICS			
NRL ID	MEAS. TOTAL CARBON FRACTION	MEAS. TOTAL CARBON %	CALC. WT %	DIFFERENCE ** (MEAS.- CALC)	MEAS. TOTAL CARBON FRACTION	MEAS. TOTAL CARBON %	CALC. WT %	DIFFERENCE *** (MEAS.- CALC)
93-67	0.677	67.7	68.49	-0.79	0.185	18.5	18.40	0.10
93-3	0.690	69.0	69.57	-0.57	0.183	18.3	18.04	0.26
93-15	0.757	75.7	76.40	-0.70	0.103	10.3	10.16	0.14
93-68	0.610	61.0	61.76	-0.76	0.215	21.5	21.44	0.06
93-50	0.745	74.5	75.14	-0.64	0.158	15.8	15.59	0.22
93-19	0.675	67.5	68.38	-0.88	0.167	16.7	16.53	0.17
93-72	0.556	55.6	56.25	-0.65	0.364	36.4	36.19	0.21
93-14	0.682	68.2	68.91	-0.71	0.199	19.9	19.68	0.22
93-71	0.615	61.5	62.25	-0.75	0.246	24.6	24.43	0.17
93-69	0.687	68.7	69.37	-0.67	0.196	19.6	19.45	0.15
93-76	0.594	59.4	60.09	-0.69	0.288	28.8	28.69	0.11
93-17	0.686	68.6	69.18	-0.58	0.220	22.0	21.75	0.25
93-51	0.737	73.7	74.19	-0.49	0.200	20.0	19.71	0.29
93-22	0.636	63.6	64.58	-0.98	0.165	16.5	16.40	0.10
93-12	0.679	67.9	67.50	0.40	0.182	18.2	17.64	0.56
93-60	0.701	70.1	70.76	-0.66	0.217	21.7	21.41	0.29
93-36	0.598	59.8	59.62	-0.82	0.218	21.8	21.65	0.15
93-27	0.696	69.6	70.22	-0.62	0.184	18.4	18.17	0.23
93-31	0.624	62.4	63.12	-0.72	0.244	24.4	24.26	0.14
93-7	0.640	64.0	64.78	-0.78	0.259	25.9	25.55	0.35
93-54	0.742	74.2	74.71	-0.51	0.192	19.2	18.85	0.35
93-78	0.665	66.5	67.25	-0.75	0.209	20.9	20.86	0.04
93-10	0.573	57.3	57.98	-0.68	0.346	34.8	34.39	0.41
93-52	0.605	60.5	61.38	-0.88	0.223	22.3	22.02	0.28
93-24	0.508	50.8	51.90	-1.10	0.199	19.9	19.88	0.02
93-9	0.642	64.2	64.92	-0.72	0.202	20.2	20.01	0.19
93-57	0.642	64.2	65.04	-0.84	0.189	18.9	18.75	0.15
93-74	0.642	64.2	64.93	-0.73	0.213	21.3	21.15	0.15
93-26	0.581	58.1	58.83	-0.73	0.248	24.8	24.70	0.10

* Measured values are the analytical data obtained by Dorn et al, Virginia Polytechnic Institute, Blacksburg, VA., using liquid chromatography/proton NMR spectrometry average compositional analysis. The calculated values are the conversion of the measured values to wt. %.

** Standard deviation of the difference for saturates is 0.24

*** Standard deviation of the difference for monocyclic aromatics is 0.11

APPENDIX D2 (Cont'd)

Compositional Analysis of Worldwide Survey I Commercial Marine Fuels

Differences Between Measured and Calculated Values For Dicyclic Aromatics and Fluorenes *

	DICYCLIC AROMATICS				FLUORENES			
NRL ID	MEAS. TOTAL CARBON FRACTION	%	CALC. WT.%	DIFFERENCE ** (MEAS.- CALC)	MEAS. TOTAL CARBON FRACTION	%	CALC. WT.%	DIFFERENCE *** (MEAS.- CALC)
87-67	0.092	9.2	8.82	0.38	0.029	2.9	2.77	0.13
87-8	0.088	8.8	8.56	0.24	0.037	3.7	3.54	0.16
87-15	0.127	12.7	12.10	0.60	0.011	1.1	1.04	0.06
87-68	0.115	11.5	11.09	0.41	0.042	4.2	4.00	0.20
87-20	0.076	7.6	7.30	0.30	0.015	1.5	1.42	0.08
87-19	0.128	12.8	12.25	0.55	0.016	1.6	1.52	0.08
87-72	0.059	5.8	5.56	0.24	0.021	2.1	2.00	0.10
87-14	0.088	8.8	8.47	0.33	0.028	2.8	2.66	0.14
87-71	0.094	9.4	9.03	0.37	0.030	3.0	2.86	0.14
87-69	0.081	8.1	7.74	0.36	0.021	2.1	2.00	0.10
87-75	0.091	9.1	8.76	0.34	0.026	2.6	2.46	0.14
87-17	0.077	7.7	7.37	0.33	0.014	1.4	1.32	0.08
87-21	0.049	4.9	4.68	0.22	0.013	1.3	1.23	0.07
87-22	0.162	16.2	15.69	0.51	0.029	2.9	2.76	0.14
87-12	0.133	13.3	12.53	0.77	0.013	1.3	1.22	0.08
87-80	0.074	7.4	7.07	0.33	0.008	0.8	0.76	0.04
87-26	0.161	16.1	15.58	0.52	0.027	2.7	2.57	0.13
87-27	0.082	8.2	7.90	0.30	0.029	2.9	2.76	0.14
87-81	0.098	9.8	9.38	0.42	0.017	1.7	1.62	0.08
87-7	0.091	9.1	8.72	0.38	0.010	1.0	0.95	0.05
87-24	0.046	4.6	4.37	0.23	0.020	2.0	1.97	0.03
87-79	0.089	8.9	8.49	0.41	0.023	2.3	2.17	0.13
87-10	0.071	7.1	6.86	0.24	0.008	0.8	0.77	0.03
87-27	0.141	14.1	13.54	0.56	0.016	1.6	1.53	0.07
87-24	0.214	21.4	20.74	0.66	0.053	5.3	5.09	0.21
87-9	0.117	11.7	11.32	0.38	0.036	3.6	3.46	0.14
87-37	0.122	12.2	11.80	0.40	0.033	3.3	3.17	0.13
87-74	0.122	12.2	11.65	0.55	0.024	2.4	2.28	0.12
87-25	0.118	11.8	11.48	0.32	0.035	3.5	3.37	0.13

* Measured values are the analytical data obtained by Dorn et al, Virginia Polytechnic Institute, Blacksburg, VA., using liquid chromatography/proton NMR spectrometry average compositional analysis. The calculated values are the conversion of the measured values to wt. %.

** Standard deviation of the difference for dicyclic aromatics is 0.14.

*** Standard deviation of the difference for fluorenes is 0.05.

APPENDIX D2 (Cont'd)

Compositional Analysis of Worldwide Survey I Commercial Marine Fuels

Differences Between Measured and Calculated Values For Phenanthrenes *

PHENANTHRENES

NRL ID	MEAS. TOTAL CARBON FRACTION	%	CALC. WT.%	DIFFERENCE ** (MEAS.- CALC)
83-67	0.016	1.6	1.52	0.08
83-8	0.003	0.3	0.29	0.01
83-15	0.003	0.3	0.29	0.01
83-62	0.018	1.8	1.71	0.09
83-30	0.006	0.6	0.56	0.04
83-19	0.014	1.4	1.32	0.08
83-72	0.000	0.0	0.00	0.00
83-14	0.003	0.3	0.29	0.01
83-71	0.015	1.5	1.43	0.07
83-69	0.015	1.5	1.43	0.07
83-76	0.001	0.1	0.00	0.10
83-17	0.004	0.4	0.38	0.02
83-31	0.002	0.2	0.19	0.01
83-22	0.006	0.6	0.57	0.03
83-12	0.012	1.2	1.12	0.08
83-80	0.000	0.0	0.00	0.00
83-36	0.006	0.6	0.58	0.02
83-27	0.010	1.0	0.95	0.05
83-81	0.017	1.7	1.61	0.09
83-7	0.000	0.0	0.00	0.00
83-34	0.001	0.1	0.10	0.00
83-78	0.013	1.3	1.23	0.07
83-10	0.000	0.0	0.00	0.00
83-23	0.016	1.6	1.52	0.08
83-24	0.025	2.5	2.40	0.10
83-9	0.003	0.3	0.29	0.01
83-37	0.013	1.3	1.24	0.06
83-74	0.000	0.0	0.00	0.00
83-26	0.017	1.7	1.61	0.09

* Measured values are the analytical data obtained by Dorn et al, Virginia Polytechnic Institute, Blacksburg, VA., using liquid chromatography/proton NMR spectrometry average compositional analysis. The calculated values are the conversion of the measured values to wt % (see Appendix D1 for conversion method)

** Standard deviation of the difference for phenanthrenes is 0.04

APPENDIX E

Determination of the Reproducibility of the SwRI Cetane Index

Based on Integrations Performed at NRL and at SwRI Using SwRI FIDs

NRL ID *	CETANE NO. (ASTM D613)	% Proton Type **					χ^2 (CH+CH2+CH3) (%)	CETANE INDEX (SwRI)	DIFFERENCE NRL - SwRI (SwRI CI)
		CH3	CH2	CH	ALPHA	AROMATICS			
83-67NRL	56.6	28.23	53.03	8.44	6.16	4.13	8046.09	60.4	0.1
83-67SW	56.6	28.46	52.98	7.95	6.41	4.10	8008.46	60.3	
83-8NRL	56.5	29.13	50.48	8.65	7.40	4.33	7729.33	54.3	0.9
83-8SW	56.5	30.17	50.00	8.10	7.54	4.19	7791.59	53.4	
83-15NRL	55.2	28.47	54.51	6.51	5.65	4.86	8008.46	60.5	1.4
83-15SW	55.2	28.63	53.53	6.64	6.22	4.98	7885.44	59.1	
83-63NRL	54.6	26.24	51.98	9.52	7.70	4.56	7699.31	58.1	0.9
83-63SW	54.6	27.75	51.45	8.67	7.51	4.62	7721.14	57.2	
83-11NRL	54.6	31.23	48.77	9.91	5.28	4.81	8083.31	52.7	0.7
83-11SW	54.6	30.41	48.22	10.41	6.03	4.93	7928.12	52.0	
83-19NRL	54.5	26.83	51.29	7.53	8.15	6.19	7335.92	56.5	1.7
83-19SW	54.5	27.46	50.15	7.16	8.66	6.57	7185.95	54.8	
83-72NRL	53.8	26.73	52.00	9.76	7.32	4.20	7830.48	59.0	0.5
83-72SW	53.8	26.94	51.67	9.44	7.50	4.44	7752.80	58.5	
83-14NRL	52.9	29.73	48.94	9.42	6.93	4.99	7759.35	53.8	0.5
83-14SW	52.9	30.16	48.64	9.24	7.07	4.89	7751.04	53.3	
83-71NRL	52.5	26.33	48.78	8.44	8.91	5.35	7318.80	53.6	0.5
83-71SW	52.5	28.77	48.49	8.22	9.04	5.48	7306.83	53.1	
83-69NRL	52.4	31.83	46.90	10.66	6.47	4.10	7999.51	51.9	0.8
83-69SW	52.4	32.28	46.56	10.32	7.14	3.70	7949.51	51.1	
83-76NRL	52.1	25.49	50.69	10.88	8.24	4.71	7579.44	57.9	-0.1
83-76SW	52.1	26.09	50.72	10.72	7.83	4.64	7661.50	58.0	

* Note: The suffix, NRL, identifies the integration data obtained at NRL. This data is based on the average of triplicate integrations.

The suffix, SW, identifies the integration data obtained at SwRI.

** Relative to the total number of protons.

APPENDIX E (Cont'd)

Determination of the Reproducibility of the SwRI Cetane Index

Based on Integrations Performed at NRL and at SwRI Using SwRI FIDs

		% Proton Type **							
NRL ID *	CETANE NO. (ASTM D613)	CH_3	CH_2	CH	ALPHA	AROMATICS	$(CH+CH_2+CH_3)^2$ (%)	CETANE INDEX (SwRI)	DIFFERENCE NRL - SwRI (SwRI CI)
87-20NRL	52.0	25.37	51.07	8.30	8.64	6.93	7130.11	56.0	0.5
87-20SW	52.0	25.61	50.91	7.62	9.15	6.71	7079.54	55.5	
87-35NRL	51.3	31.99	47.37	10.21	5.94	4.49	8022.78	53.0	0.7
87-35SW	51.3	32.67	46.89	10.00	5.78	4.67	8020.99	52.3	
87-17NRL	50.4	29.83	45.69	12.00	7.63	4.80	7668.50	50.4	-0.2
87-17SW	50.4	30.55	45.66	11.90	6.75	5.14	7763.37	50.6	
87-21NRL	50.3	31.26	46.50	11.82	6.22	4.20	8024.58	52.5	-0.4
87-21SW	50.3	31.74	46.85	11.34	6.05	4.03	8087.40	52.9	
87-22NRL	48.8	27.44	46.48	10.30	9.04	6.73	7093.01	49.7	0.5
87-22SW	48.8	28.70	46.30	9.26	8.95	6.79	7099.75	49.2	
87-12NRL	48.8	30.99	44.58	11.94	7.29	5.20	7658.00	49.2	1.2
87-12SW	48.8	31.40	44.06	11.35	8.18	5.01	7535.98	48.0	
87-30NRL	48.7	34.64	43.34	11.75	6.18	4.09	8051.47	48.1	1.0
87-30SW	48.7	34.09	42.68	12.12	7.07	4.04	7901.43	47.1	
87-26NRL	48.7	28.13	47.63	10.95	8.05	5.23	7518.62	52.6	0.5
87-26SW	48.7	28.31	47.46	10.17	8.23	5.33	7471.87	52.1	
87-27NRL	48.5	27.31	46.41	11.12	9.10	5.56	7282.92	50.6	0.9
87-27SW	48.5	28.82	46.18	10.00	9.71	5.29	7225.00	49.7	
87-31NRL	47.9	33.60	42.42	12.61	7.14	4.23	7855.28	47.0	1.1
87-31SW	47.8	33.50	41.75	12.75	7.75	4.25	7744.00	45.9	
87-7NRL	47.7	30.33	45.97	9.89	8.62	5.23	7420.10	49.9	1.8
87-7SW	47.7	30.25	44.82	9.80	9.30	5.32	7202.92	48.1	

* Note: The suffix, NRL, identifies the integration data obtained at NRL. This data is based on the average of triplicate integrations.

The suffix, SW, identifies the integration data obtained at SwRI.

** Relative to the total number of protons.

APPENDIX E (Cont'd)

Determination of the Reproducibility of the SwRI Cetane Index

Based on Integrations Performed at NRL and at SwRI Using SwRI FIDs

NRL ID *	CETANE NO. (ASTM D613)	% Proton Type ** CH3	CH2	CH	ALPHA	AROMATICS	$(CH+CH_2+CH_3)^2$ (%)	CETANE INDEX (SwRI)	DIFFERENCE NRL - SwRI (SwRI CI)
83-34NRL	47.3	34.53	45.47	10.69	5.47	3.84	8224.68	50.2	0.0
83-34SW	47.3	33.65	45.59	11.22	6.21	3.34	8181.20	50.2	
83-78NRL	47.1	32.61	42.52	14.09	7.22	3.57	7960.21	47.9	1.2
83-78SW	47.1	33.75	41.81	13.10	7.30	4.03	7860.60	46.7	
83-10NRL	46.8	36.52	32.55	16.59	9.74	4.60	7337.64	33.4	0.9
83-10SW	46.8	36.88	31.95	16.36	10.13	4.68	7257.34	32.5	
83-16SW	45.7	21.45	48.75	4.18	13.93	11.70	5532.38	48.9	-1.0
83-16NRL	45.7	21.26	49.41	4.33	13.29	11.71	5625.00	49.9	
83-22NRL	47.6	25.43	45.35	9.30	11.95	7.97	6412.81	49.6	1.2
83-22SW	47.6	25.67	44.54	9.20	12.36	8.33	6290.08	48.4	
83-24NRL	42.8	23.58	43.71	9.75	13.10	9.85	5935.16	47.1	-0.3
83-24SW	42.8	24.77	44.04	9.17	12.54	9.48	6080.88	47.4	
83-11NRL	40.9	36.53	32.75	17.17	9.24	4.31	7473.60	34.6	0.9
83-11SW	40.9	38.44	32.41	15.83	9.05	4.27	7513.42	33.7	
83-9NRL	54.3	28.12	51.25	9.27	6.98	4.39	7857.05	57.7	0.1
83-9SW	54.3	28.49	51.28	9.12	7.12	3.99	7901.43	57.6	
83-37NRL	50.2	28.96	49.33	8.74	8.02	4.93	7577.70	53.1	0.8
83-37SW	50.2	29.03	48.68	9.09	8.21	4.99	7534.24	52.3	
83-74NRL	48.6	27.70	45.73	12.98	8.34	5.25	7466.69	51.0	1.3
83-74SW	48.6	28.20	45.86	12.50	9.01	5.23	7354.78	49.7	
83-26NRL	47.8	30.60	46.33	9.79	8.29	4.50	7697.33	46.8	1.1
83-26SW	47.8	32.24	46.10	9.87	8.06	4.53	7640.51	45.7	

* Note: The suffix, NRL, identifies the integration data obtained at NRL. This data is based on the average of triplicate integrations.

The suffix, SW, identifies the integration data obtained at SwRI.

** Relative to the total number of protons.

END

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